EASTMAN CHEMICAL COMPANY
P. O. Box 511
Kingsport, TN 37662

FAP 2197

RUMEN PROTECTED AMINO ACIDS FOR BEEF CATTLE

May 14, 1990

HEADING H

TABLE OF CONTENTS OF ENVIRONMENTAL ASSESSMENT
AND ENCLOSURES
for
Rumen Protected Amino Acids for Beef Cattle

<u>Environmental Assessment</u> (May 14, 1990)

HEADINGS

Heading H, Enclosure 1, Emission and waste treatment permits issued by the Arkansas Department of Pollution Control and Ecology to Arkansas Eastman Company. NPDES Permit issued by the Environmental Protection Agency to Arkansas Eastman Company.

Heading H, Enclosure 2, NPDES permit issued by the Tennessee Department of Health and Environment to the Tennessee Eastman Company. Emission and waste treatment permits issued by the Tennessee Department of Health and Environment to Tennessee Eastman Company.

Heading H, Enclosure 3, Talc, page 450.3 from Food Chemical News Guide, Food Chemical News, Inc. Washington, D.C. (1978).

Heading H, Enclosure 4, Eastman's letter of April 29, 1982, Summarizing Proposed Environmental Testing for Poly(2-vinylpyridine-co-styrene).

Heading H, Enclosure 5, Copy of published article "The Biology of Talc," G. Y. Hildick-Smith, British Journal of Industrial Medicine, 33:217-229 (1976).

Heading H, Enclosure 6, Part A, "General Solubility of Poly(2-vinylpyridine-co-styrene)," Industrial Laboratory, Eastman Kodak Company, Rochester, New York, July 17, 1984.

Heading H, Enclosure 6, Part B, "Specific Buffer Solubility of Poly(2-vinylpyridine-co-styrene)," Health and Environment Laboratories, Eastman Kodak Company, Rochester, New York, June 9, 1984.

Heading H, Enclosure 6, Part C, "Soil Metabolism Test on Poly(2-vinylpyridine-co-styrene)," Health and Environment Laboratories, Eastman Kodak Company, Rochester, New York, August 23, 1984.

Heading H, Enclosure 6, Part D, "Shake-Flask Biodegradation, Poly(2-vinylpyridine-co-styrene)," Health and Environment Laboratories, Eastman Kodak Company, Rochester, New York, August 21, 1984.

Heading H, Enclosure 6, Part E-1, "Determining the Effects of Poly(2-vinylpyridine-co-styrene) on Plant Growth," Health, and Environment Laboratories, Eastman Kodak Company, Rochester, New York, July 3, 1984. (Revised August 26, 1986).

Heading H, Enclosure 6, Part E-2, "Determining the Effects of Poly(2-vinylpyridine-co-styrene) on Plant Growth," Health, and Environment Laboratories, Eastman Kodak Company, Rochester, New York, May 3, 1990.

Heading H, Enclosure 6, Part F, "Secondary Waste Treatment Compatability, Poly(2-vinylpyridine-co-styrene)," Health and Environment Laboratories, Eastman Kodak Company, Rochester, New York, August 9, 1984. (Revised July 25, 1985).

Heading H, Enclosure 6, Part G, "Earthworm Toxicity Study of Poly(2-vinylpyridine-co-styrene), in Artificial Soil," Biospherics Incorporated, Rockville, MD, July 1984.

Heading H, Enclosure 6, Part H, Biospherics's letter commenting on the earthworm study in Heading H, Enclosure 6, Part G, Biospherics Incorporated, Rockville, MD, April 8, 1985.

Environmental Assessment for Rumen Protected Amino Acids for Beef Cattle

1. Date: May 14, 1990

2. Name of Petitioner: Eastman Kodak Company
   Eastman Chemicals Division

3. Address: P.O. Box 511
   Kingsport, Tennessee 37662

4. Description of the Proposed Action

   a. The Purpose and Need for the Action

   The purpose of this petition is to secure a food additive regulation which will enable the petitioner to offer the amino acids, methionine and lysine, for beef cattle in feedlots and farmer-feeder operations in a form which will protect these articles from destruction in the rumen but will, by use of a specialized polymeric substance, poly(2-vinylpyridine-co-styrene) (copoly VP/ST), permit their transport through the rumen into the abomasum where the polymer loses its integrity releasing the nutrients for absorption. The polymer is produced by classical emulsion polymerization procedures, dried, and applied by suitable means to the nutrient to be protected.

   b. The Locations Where the Product Will Be Produced

   The polymer will be produced and purified to meet established specifications at Arkansas Eastman Company, Batesville, Arkansas, and employed in the production of rumen-protected lysine and methionine (RPAA) at Tennessee Eastman Company, Kingsport, Tennessee, the petitioner's production affiliates in the Eastman Kodak Company organization.

   c. The Locations Where the Product Will be Used

   The RPAA will be marketed throughout the United States and abroad for use as a nutrient supplement in the feed of beef cattle in feedlots.

d. The Location Where the Product Will Be Disposed Of

The polymer is not absorbed by the ruminant animal but is excreted, chemically unchanged, in the feces with other waste products.

e. The Types of Environments Present at Locations Identified at b, c, and d

The environment at Arkansas Eastman Company, where copoly VP/ST will be produced, is characteristic of a highly diversified chemical manufacturing facility. The environment at Tennessee Eastman Company, where copoly VP/ST will be used in the manufacture of RPAA, is characteristic of a highly diversified chemical and plastic manufacturing facility. Consequent activities involving RPAA will occur wherever cattle are fed in feedlots for production of meat. This includes farmer-feeders and commercial feedlots. Feces generated by these animals will be distributed to the terrestrial environment as manure according to practices employed in the cattle feeding industry.

5. Identification of Chemical Substances Subject to the Proposed Action:

a. Introduction

Rumen-Stable Amino Acids will be supplied as pellets produced from methionine and lysine with the adjuvant substances, food grade talc, edible fatty acids, i.e., stearic acid, and copoly VP/ST. These pellets will be coated or enrobed with a formulation containing copoly VP/ST, talc, and edible fatty acids.

A typical rumen-protected amino acid preparation has the following approximate composition:

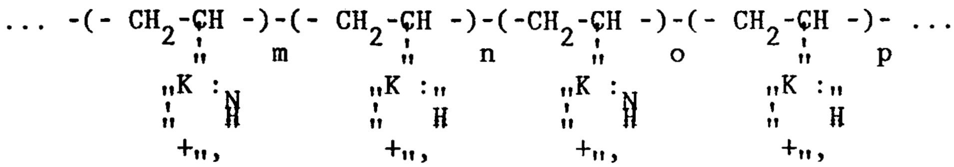
Component	Percent
Lysine Hydrochloride	50.85
Methionine	12.29
Stearic Acid	12.39
Talc	19.32
Copoly VP/ST	5.15

The final product will contain less than 10.3 ppb each of the monomers, styrene and 2-vinylpyridine. (One specification for the polymer is that it contain less than 200 ppb of each monomer.) The value 10.3 is the fraction of the polymer in the final product times 200 ppb (0.0515*200 ppb).

b. Poly(2-vinylpyridine-co-styrene)

CAS Registry Number: 24980-54-9

Structural formula:



The copolymer is a random arrangement of repeating units derived from 2-vinylpyridine and styrene. The probabilities of various sequences along the polymer chain are determined by the relative reactivities of the monomers and their relative concentrations during polymerization. In the final polymer, the 2-vinylpyridine:styrene ratio is between 65:35 and 80:20.

Molecular weight: 100,000-500,000

Solubility: <0.1% in corn oil; between 0.1% and 1.0% in acetone, dimethyl sulfoxide, octanol, tetahydrofuran, and p-dioxane; in water, 92.7 ppb at pH 5, 88.6 ppb at pH 7, and 185.6 ppb at pH 9.[1,2]

Vapor pressure: Estimated by the CHEMEST[3] Program to be 1.94×10^{-26} Torr (Appendix I).

Octanol-water partition coefficient[2]: 10^4 to 10^5.

Soil absorption coefficient: 1.08×10^5 (Appendix I).

Ultraviolet absorptivity: 23.96 at 262 nm.[4]

c. Talc[5]

CAS Registry Number: 14807-96-6

Chemical composition: native hydrous magnesium silicate $(Mg_3Si_2O(OH)_4)_{10}$

Physical form: finely powdered solid.

Solubility: insoluble in water, cold acids or alkalies.

d. Stearic Acid (as an example of an edible fatty acid)[6]

CAS Registry Number: 57-11-4

Structural formula: $CH_3(CH_2)_{16}COOH$

Solubility: very slightly soluble in water; ¦1% soluble in alcohol, acetone, chloroform, carbon disulfide and other organic solvents.

Boiling point: 383°C.

Melting point: 69-70°C.

e. Methionine[7]

CAS Registry Number: 63-68-3

Structural formula: $CH_3SCH_2CH_2CH(NH_2)COOH$

Solubility: in water, 18.8 g/L at 25°C, 33.81 g/L at 50°C; very slightly soluble in 95% alcohol; insoluble in ether.

Melting point: 281°C (dec.)

f. Lysine Hydrochloride[8]

CAS Registry Number: 56-87-1

Structural formula: $NH_2(CH_2)_4CH(NH_2)COOH$

Solubility: freely soluble in water; very slightly soluble in alcohol; insoluble in ether.

Melting point: 210-224.5°C (dec.)

g. Styrene[9]

CAS Registry Number: 100-42-5

Structural formula: $C_6H_5CH=CH_2$

Solubility: in water, 280 mg/L at 15°C, 300 mg/L at 30°C, 400 mg/L at 40°C.

Octanol-water partition coefficient: 891 (Log K_{ow} = 2.95) (Appendix 2)

Soil absorption coefficient: 573 (Appendix 2)
Ultraviolet absorbance: Molar extinction coefficient = 15140 at 245nm in ethanol.[4]

Boiling point: 145.2°C

Vapor pressure: 10 mm at 30.8°C

Melting point: -30.63°C

h. 2-Vinylpyridine[10]

CAS Registry Number: 100-69-6

Structural formula: $C_5H_4NCH{=}CH_2$

Solubility: In water, 27.5 g/L at 20°C; very soluble in alcohol, acetone, ether, and other organic solvents.

Octanol-water partition coefficient: 63 (Log K_{ow} = 1.80) (Appendix 3)

Soil absorption coefficient: 47 (Appendix 3)

Ultraviolet absorbance: Molar extinction coefficient = 12600 at 238nm in ethanol.[4]

Boiling point: 159-160°C

Vapor pressure: 10 mm at 44.5°C

6. Introduction of Substances Into the Environment:

a. Assumptions for amounts of materials entering the environment.

1). RPAA will be marketed only to commercial feedlots and farmer-feeder operations where beef cattle are confined to pens.

The economics of production of a sophisticated product such as RPAA and the growth of range cattle are basically incompatible. In addition, there is no way to distribute RPAA to range cattle because RPAA's somewhat fragile coating can be ruptured and the protecting effect lost if it is not properly handled. Therefore, a basic assumption for the market size and consequently the amount of any given component entering the environment is based on RPAA being fed only to feedlot or farmer-feeder cattle.

2). Nationwide, approximately 27 million cattle were fed in feedlots or farmer-feeder operations in 1989[11] (Appendix 4).

This number was obtained as follows:

In 1989, the 13 states that the USDA Economics Statistics & Cooperatives Service annually reports marketed 22,955,000 head. The number of cattle marketed annually for the nation is not available but can be calculated. As of January 1, 1990, these 13 states had 9,943,000 head on feed and the nation as a whole had 11,626,000 on feed. The ratio of the national figure and the value for the 13 states is 1.17. The annual figure for the 13 states of 22.96M head can thus be adjusted by multiplying by this ratio to give a national figure.[11] That is 22.96M*11.626M/9.943M = 26.85M head marketed nationwide.

3). All cattle in the feedlot/farmer-feeder population use RPAA.

4). The amount of RPAA fed per head per day is 20 g.

In feeding trials 20 g of RPAA per head per day gave the optimum improvement in weight or feed conversion with no further improvement with more feed.[12] A much more likely amount to be fed in this extremely competitive industry is 15 g per head per day because this lower level is more cost effective. Therefore 20 g per head per day is a reasonable estimate.

5). RPAA will be fed for 158 days.

From the above USDA figures of 9.943M head on feed in 13 states at any one time (Jan. 1) and the total slaughtered of 22.96M head, the number of cycles is 2.31 or 158 days/cycle. (22.96/9.943 = 2.31, 365/2.31 = 158).

b. Controls Used at the Manufacturing Sites:

Manufacture of Copoly VP/ST

Copoly VP/ST is produced at Arkansas Eastman Company in Batesville, Arkansas, by emulsion polymerization of 2-vinylpyridine and styrene. These facilities operate under an NPDES permit issued by the United States Environmental Protection Agency (EPA) and emission and waste treatment permits issued by the Arkansas Department of Control and Ecology.[13] The EPA NPDES permit expired on June 30, 1981. On December 30, 1980, Eastman filed a request that extended this permit, a copy of the request is included in Enclosure 1. An official extension has not been issued. However, under the uniform Administrative Procedures Act, once timely application for permit renewal has been made, a permittee may continue to discharge under an existing permit until a new permit has been issued.

Air emissions will be controlled by high efficiency waste scrubbers to minimize the emission of volatile organic chemicals and meet the limits designated in the NPDES permit. Estimates from Arkansas Eastman Company indicate approximately 0.23 pound of VOC per day of production. Duration of emissions, which consists of monomeric 2-vinylpyridine, styrene, acetone, and methanol will probably be continuous when production of copoly VP/ST becomes commercial.

The effluent from the manufacturer of copoly VP/ST (including 2-vinylpyridine, styrene, sodium hydroxide, isopropyl alcohol, oleic acid, sodium sulfate, and sodium chloride) will be discharged to existing company waste treatment facilities operating under an existing permit issued by the Arkansas Department of Control Ecology.[13] Copoly VP/ST will not be degraded by the Arkansas Eastman waste treatment process and will finally be disposed of by spray irrigation on company property along with other treated waste water effluents. A description of the Arkansas wastewater treatment system follows.

At Arkansas Eastman Company, the wastewater treatment system begins with a 14 million gallon diversion basin. This basin is designed to protect the biological system by intercepting any wastes entering the wastewater treatment piping system which are not within proper treatment specifications. Wastes retained in the diversion basin can be gradually fed to the remainder of the wastewater treatment plant in a manner which prevents a system upset. Wastes within proper treatment specifications enter an equalization basin with a one-day retention time. Here, peak flows and organic loadings are equalized and pH of the wastewater is adjusted prior to biological treatment.

The biological treatment system consists of two extended aeration activated sludge basins with a combined volume of 22.5 million gallons followed by two clarifiers. One basin is equipped with subsurface aerators and the other basin is equipped with mechanical surface aerators. Both aeration systems provide dissolved oxygen to the microorganisms engaged in degrading the waste. Under average flow conditions, each basin provides a retention time in excess of 10 days. This lengthy retention time produces efficient removal of organics as well as nitrification. Following aeration, biological solids are removed from the treated wastewater in either a 120- or a 75-foot diameter clarifier.

The majority of the concentrated solids are returned to the aeration basin in order to maintain the required population of microorganisms. Excess solids receive treatment by aerobic sludge digestion prior to disposal by spray irrigation at a site located on Company property.

The effluent flows from either clarifier to a polishing basin and then combines with treatment sanitary wastes and coal ash settling basin effluent to form Outfall 002. Outfall 002, in turn, combines with the effluent from a large cooling water holding pond, Outfall 001, to form the total plant effluent which flows through a channel to the White River.

The flow in Outfall 002 usually averages about 1.0 - 1.5 million gallons per day (MGD) and the total Arkansas Eastman discharge, including the cooling water holding pond effluent, averages about 14 MGD. In terms of the average flow in the White River at Batesville, the treated wastewater averages 0.01 percent of the river flow and the total Arkansas Eastman discharge averages 0.2 percent of the flow.

Manufacture of RPAA

The finished rumen protected amino acid product is manufactured at Tennessee Eastman Company in Kingsport, Tennessee. This facility operates under a NPDES permit issued by the United States Environmental Protection Agency to Tennessee Eastman Company and an operating permit issued by the Tennessee Department of Health and Environment.[14]

Copoly VP/ST as a dry powder is blended with edible fatty acids and the blend is combined with the appropriate amino acids and compounded into nutrient cores. Compounding is by extrusion of the dry components followed by cutting and rounding. Fines produced as a result of this operation are retained on filters for collection and incineration. The cores are coated with an acetone/methanol solution of copoly VP/ST and stearic acid containing suspended talc.

Air emissions from core production and coating operations at Tennessee Eastman Company are included in the operating permit previously cited.[14]

The effluent from the manufacture of RPAA may contain traces of acetone, methanol, copoly VP/ST, edible fatty acids, and talc. The effluent from this process is diverted to the waste treatment facility operating under the above permit. Copoly VP/ST is not expected to be degraded in the waste treatment process and will finally be disposed of by incineration.

c. Quantity and Concentration of Substances Expected to Enter the Environment through Feeding RPAA to Beef Cattle:

The purpose of RPAA is to deliver the active ingredients, methionine and lysine, past the rumen of beef cattle in feedlots and farmer-feeder operations where upon the polymer (copoly VP/ST) coating and matrix loses its integrity releasing the protected nutrient.

Assumptions:

1). Number of cattle in feedlots/year = 27,000,000 nationwide.
2). Amount of RPAA fed = 20 g/head/day.
3). Feeding period = 158 days.

4). The two amino acids and the edible fatty acids used in the production of RPAA is absorbed by the ruminant.

5). All copoly VP/ST, talc and trace quantities of styrene and 2-vinylpyridine enter the environment in the feces of beef cattle fed RPAA.

6). Manure application rate on a dry basis is 10.23×10^3 kg/acre/year.

According to Dr. Charles Strasia, Oklahoma State University Extension Center, the moisture content of air-dry manure that is normally spread is 25%.[15] His estimated application rates agree with the value of 10 to 15 air-dried tons per acre that is given in The Feedlot.[16] The calculation for manure application rate on a dry basis is: 15 air-dried tons/acre x .75 (the fraction of dry manure in air-dried manure) x 2000 lb/ton/2.2 lb/kg gives the amount of manure per acre on a dry basis in kilograms.

7). Feedlot beef cattle produce approximately 28.2 kg of manure per day that is about 65% moisture or 9.9 kg of dry manure per head per day.[15]

8). Weight of an acre-furrow[17] = 9.09×10^5 kg.

The composition of RPAA given earlier in this Environmental Assessment is repeated here for the convenience of the reader.

Component	Percent
Lysine Hydrochloride	50.85
Methionine	12.29
Stearic Acid	12.39
Talc	19.32
Copoly VP/ST	5.15

The final product will contain less than 10.3 ppb each of the monomers, styrene and 2-vinylpyridine. (One specification for the polymer is that it contain less than 200 ppb of each monomer.) The value 10.3 ppb is the fraction of the polymer in the final product times 200 ppb (0.0515*200 ppb).

Quantity and Concentration of Copoly VP/ST per year:

Fraction Copoly VP/ST in RPAA = 0.0515

Quantity of Copoly VP/ST = 9.7M lb/year

(27×10^6 head x 20 g RPAA/head/day/454 g/lb x 158 days x 0.0515 = 9.7M lb/year)

Quantity of RPAA = 188.4M lb/year

(9.7M lb/year/0.0515 = 188.4M lb/year)

Concentration in manure = 1.0×10^{-4} kg/kg of manure

(0.0515 x 20 g/head/day/1000 g/kg/9.9 kg manure/head/day = 1×10^{-4} kg/kg manure)

Concentration in soil = 1.17×10^{-6} kg/kg soil or 1.17 mg/kg

(1.0×10^{-4} kg copoly VP/ST/kg manure x 10.23×10^3 kg manure/acre/year/9.09×10^5 kg/acre-furrow = 1.17×10^{-6} kg/kg soil or 1.17 mg/kg)

Quantity and Concentration of Talc per year:

Fraction of Talc in RPAA = 0.1932%

Quantity = 36.3M lb/year

(27×10^6 head x 20 g/head/day/454 g/lb x 158 days x 0.1932 = 36.3M lb/year)

Concentration in manure = 3.9×10^{-4} kg talc per kg manure

(0.193 x 20 g/head/day/1000 g/kg/9.9 kg manure/head/day = 3.9×10^{-4} kg/kg manure)

Concentration in soil = 4.4×10^{-6} kg talc/kg of soil

(3.9×10^{-4} kg talc/kg manure x 10.23×10^3 kg manure/acre/year/9.09×10^5 kg/acre-furrow = 4.4×10^{-6} kg/kg of soil)

Quantity and Concentration of Styrene and 2-Vinylpyridine each per year:

Concentration of styrene and 2-vinylpyridine each in RPAA = 10.3 ppb.
Quantity = 1.9 lb styrene and 2-vinylpyridine each/year

(27×10^6 head x 20 g/head/day/454 g/lb x 158 days x 10.3×10^{-9} = 1.9 lb of each monomer)

Concentration in manure = <u>2.1×10^{-11} kg (20ppt) styrene and 2-vinylpyridine each per kg of manure</u>

($10.3 \times 10^{-9} \times 20$ g/head/day/1000 g/kg/9.9 kg manure/head/day) = 2.1×10^{-11} kg/kg manure)

Concentration in soil = <u>2.4×10^{-13} kg (0.24 ppt) styrene and 2-vinylpyridine each/kg of soil</u>

(2.1×10^{-11} kg/kg manure x 10.23×10^{3} kg manure/acre/year/9.09×10^{5} kg/acre-furrow = 2.4×10^{-13} kg/kg of soil or 0.24 parts per trillion)

7. <u>Fate of Emitted Substances in the Environment</u>

Since the expected route of introduction of copoly VP/ST into the environment is through excretion by the target animal, the petitioner conducted several studies of the fate of this food additive in the environment. Reports of specific fate tests, identified below, along with the protocols submitted to the administration for acceptance prior to initiating the tests, are included as <u>Heading H, Enclosure 6, Parts A-G</u>.

<u>Styrene and 2-Vinylpyridine Fate:</u>

Styrene and 2-vinylpyridine have appreciable vapor pressures, 10mm at 30.8°C and 44.5°C respectively. Therefore, the 1.9 lb/year (0.24 ppt) of each that is expected to enter the environment is expected to volatilize into the air. Assuming that the monomers are continuously released from a single point source, and utilizing the technique for approximating the impact of area sources outlined in Turner's workbook[18], the predicted maximum ambient concentrations of styrene and 2-vinylpyridine are 57 ppt and 61 ppt respectively. This methodology predicts the highest possible concentration of monomers in ambient air.

These maximum concentrations were calculated as follows:

An approximation of an area source's ambient impact can be made by combining all of the emissions in a given area and treating this area as a source having an initial horizontal standard deviation, s_{yo}. A virtual distance, xy, can then be found that will give this standard deviation. Values of xy will vary with atmospheric stability. Then equations for point sources may be used, determining s_y as a function of x + xy.

This procedure treats the area source as a cross-wind line source with normal distribution, a fairly good approximation for the distribution across an area source. The initial standard deviation for a square area source can be approximated by $s_{yo} = s/4.3$, where s is the length of a side of the area.

The following calculations illustrate the application of this technique to predict the maximum downwind concentrations of styrene and 2-vinylpyridine:

area of source = 4.1×10^6 acres.
= 1.8×10^{11} sq. ft.

assuming the area is square;

length of side, s = 4.2×10^5 ft.
= 1.3×10^5 meters.

emission rate, q = 0.26 g/s for styrene.
= 0.28 g/s for 2-vinylpyridine.

Note: Emission rates are based on convection mass transfer calculations.

$s_{yo} = s/4.3 = 3.0 \times 10^4$ meters.

maximum ground level concentration,
$C_{max} = q/(3.14159 \times m \times s_{yo} \times s_{zo}$.

where:
q = emission rate, g/s.
m = wind speed, m/s.
s_{yo}, s_{zo} = horizontal and vertical standard deviations of plume concentration distribution, m.

assuming a neutral atmospheric stability and a 5 mph wind;

s_{zo} = 5 meters.
m = 2.24 m/s.

C_{max} = 57 ppt for styrene.
= 61 ppt for 2-vinylpyridine.

Copoly VP/ST Fate in Specific Compartments:

a. Air

Copoly VP/ST is a polymer having a molecular weight in the range 100,000 to 500,000, and an estimated vapor pressure of 1.94×10^{-26} Torr. Therefore, it is not expected to enter the air during manufacture or use.

b. Aquatic Ecosystems

Because copoly VP/ST has a low solubility in water and because of facilities for wastewater treatment at Arkansas Eastman Company and Tennessee Eastman Company, the production of copoly VP/ST and the manufacture of RPAA will not result in any significant release of copoly VP/ST to the aquatic environment. Similarly, the use and disposal of copoly VP/ST and RPAA will not result in any direct release of copoly VP/ST to the aquatic environment. The solubility and bioconcentration information that follow indicate that no more than trace quantities of copoly VP/ST are likely to enter the aquatic environment and that no subsequent bioconcentration is expected to occur.

Organic Solvent Solubility

The petitioner has examined the general solubility of copoly VP/ST in distilled water, corn oil, acetone, octanol, dimethylsulfoxide (DMSO), tetrahydrofuran (THF), and p-dioxane. Visual inspection was used to determine whether or not copoly VP/ST was completely dissolved by each of these seven common solvents following sonication of 0.1, 1.0, and 10% mixtures of polymer in these solvents. The polymer has a low solubility (<0.1%) in distilled water, corn oil, and acetone; it has a moderate solubility (0.1% <S <1.0%) in DMSO, octanol, THF, and p-dioxane.[1]

Aqueous Solubility

In a more definitive study,[2] the solubility of copoly VP/ST was measured in aqueous solutions at pH values of 5, 7, and 9. A sample of (^{14}C) copoly VP/ST having the same specifications as commercial copoly VP/ST was used. (^{14}C)Copoly VP/ST was added to twelve 125-mL Hypo-Vials*. Six of the vials received approximately 50 mg each of (^{14}C)copoly VP/ST and six received approximately 100 mg each. Two vials at each weight received either 50 mL acetate buffer (pH 5), 50 mL phosphate buffer (pH 7), or 50 mL borate buffer (pH 9). One sample of each weight at each pH was sonicated for 0.25 minutes and one sample of each weight at each pH was sonicated for 30 minutes. All samples were then incubated with shaking overnight at 25°C. Each sample was then centrifuged at 9,000 x g for ten minutes. One mL (in triplicate) of the aqueous phase was mixed with 10 mL of Eastman Ready-to-Use II* scintillation cocktail. The samples were cooled and dark adapted for four hours, then counted for 20 minutes each in a Packard Model 4530 Liquid Scintillation Spectrometer. A calibration curve was prepared using samples of (^{14}C)copoly VP/ST in pyridine. Using linear regression analysis, the equation for the calibration curve was:

$$y = 1.0137\,x - 40.55$$

where y = net sample dpm and x = (^{14}C)copoly VP/ST concentration. The correlation coefficient = 0.9987. The net sample dpms were inserted into this equation and solved for the concentration of copoly VP/ST.

The mean solubility for (^{14}C)copoly VP/ST was determined to be as follows: pH 5, 92.7 ppb; pH 7, 88.6 ppb; and pH 9, 185.6 ppb.[2] Copoly VP/ST is not expected to leach from soil because of the extremely low aqueous solubility, an octanol-water partition coefficient of 10^4 to 10^5, and a soil absorption coefficient estimated to be approximately 10^5 (Appendix 1).

Bioconcentration Potential

A large octanol-water partition coefficient may indicate that a compound will bioaccumulate in organisms in the environment. However, this coefficient is not considered to be an accurate indication of bioconcentration potential for copoly VP/ST. First, it is known that high molecular weight compounds are not appreciably absorbed in the G. I. tract. For example Tagesson, et al, studied the intestinal permeability of the water soluble poly(ethylene glycol) (PEG) in the molecular weight range 634-1338. An exponential decrease was observed with the highest molecular weight showing less than 2% absorption.[19] The much higher molecular weight for copoly VP/ST should further decrease its absorption. Another factor that should cause a very low or negligible passage of this polymer through cell membranes is its extremely low aqueous solubility.

These arguments are supported by the results of a study in which carbon-14 labeled copoly VP/ST was fed to rats.[20] In this study, instead of 2-vinylpyridine, 2-methyl-5-vinylpyridine with similar molecular weight, mol. wt. distribution, and chemical and physical properties was used. The FDA accepted data from this polymer as being applicable to the 2-vinyl case. This polymer was also called copoly VP/ST.

Carbon-14 labeled copoly VP/ST was dissolved in acetone and administered by gavage to male Charles River rats (N=3) at a dose of 100 mg/kg of body weight. Essentially all of the radioactivity administered was recovered in the feces within 72 hours after dosing. Radioactivity in the carcass, urine, blood or tissues, with the exception of the gastrointestinal tract, was below the limit of detection. The total recovery of carbon-14 ranged from 100 to 107% of the administered dose. The analysis of fecal extracts by thin layer chromatography suggested that the radioactive material in the feces was similar to that of an authentic sample of carbon-14 labeled polymer. These findings suggest copoly VP/ST was stable in the gastrointestinal tract, was not absorbed, and was eliminated in the feces unchanged.[20]

Therefore, the potential for copoly VP/ST to bioconcentrate is considered to be low.

Biodegradation

A shake-flask biodegradation study, designed to estimate the extent to which copoly VP/ST will be degraded in surface waters and by biological waste treatment microorganisms, was conducted.[21]

The microbes used in this study were from a laboratory culture and were acclimated to copoly VP/ST for 21 days prior to the start of the test. Acclimation consisted of introducing into the culture (every two to three days) progressively less food and progressively more polymer. After acclimation, quintuplicate samples of about 11 mL each were prepared in biometer flasks in the following manner.

Treatment

Sample	BSM	SA	TC	THF	Inoc.	Gluc.
Test Solution	10 mL		50 mL		1 mL	
Sterile Control	10 mL	1 mL	50 mL			
Negative Control	10 mL			50 mL	1 mL	
Positive Control	10 mL				1 mL	130 mL

BSM = Basal Salt Medium Solution
SA = 0.05% Sodium Azide Solution
TC = Test Chemical Solution of 202.81 mg (^{14}C)copoly VP/ST in 10 mL of THF
THF = Tetrahydrofuran
Inoc.=Microbes acclimated to copoly VP/ST
Gluc.=(^{14}C)glucose

The flask assemblies were placed on a shaker and kept in the dark at 22 ± 2°C for 28 days. A scintillation vial attached to each flask trapped $^{14}CO_2$ that was released. The vials were replaced and $^{14}CO_2$ was assayed on days 1, 3, 7, 14, 21, and 28. About 30% of the (^{14}C)glucose in the positive control was metabolized to $^{14}CO_2$. The total $^{14}CO_2$ that was obtained in the polymer test flasks averaged about 0.006%.

On day 28 of the test, the contents of each biometer flask were removed and filtered. The clear filtrate was assayed for radioactivity. The filtered solids were extracted with pyridine, then dried, combusted, and the combustion product (i.e., CO_2) assayed for radioactivity. Finally, the pyridine extract was assayed for radioactivity. Almost all (97% to 98%) of the radioactivity was found in the pyridine extract of the filter paper and solids.

To determine if there was any evidence of primary degradation of (^{14}C)copoly VP/ST by the microorganisms, samples of the pyridine extracts also were assayed using gel permeation chromatography. The chromatograms showed no evidence of (^{14}C)copoly VP/ST biodegradation.[21]

Based on these data, it is reasonable to conclude that copoly VP/ST is quite resistant to biodegradation by wastewater treatment organisms (<0.006%) even if they are acclimated to this polymer.

c. Terrestrial Environment

Biodegradation of Copoly VP/ST in Soil

A soil metabolism test was performed to determine the extent to which copoly VP/ST will biodegrade in the terrestrial environment.[22] Three different soil types were collected and used in this study. These soils were identified as sandy loam, loam, and loamy sand. Each of the three soil types were brought to 75% of field moisture capacity and used in the following fashion in this study. Twelve samples of approximately 2.5 g of each soil type were added to 50 mm x 10 mm cellulose extraction thimbles. The samples were divided into four groups of three each by treating with: (1) 50 mL of a test chemical solution of (^{14}C)copoly VP/ST in tetrahydrofuran (THF); (2) 50 mL of THF (negative control); (3) 50 mL of the test chemical solution of (^{14}C)copoly VP/ST in THF to soil which was autoclaved at 121°C (sterile control); or (4) 130 mL of (^{14}C)glucose (positive control). Each thimble was placed in a 50-mL biometer flask. The biometer flask assemblies were placed on a shaker in the dark at 22 ± 1°C for 28 days. A scintillation vial, containing 1 mL of diethanolamine attached to each flask, trapped the $^{14}CO_2$ released. The vials were removed and assayed on days 3, 7, 14, 21, and 28 and fresh vials containing diethanolamine were attached on days 3, 7, 14, and 21.

Cumulative measurements of $^{14}CO_2$ evolution were made. From 54% to 60% of the (^{14}C)glucose in the positive control was metabolized to $^{14}CO_2$. The total $^{14}CO_2$ that was released in the polymer test flasks ranged from 0.0015% to 0.0021%.

On day 28, the solids in each biometer flask were extracted with pyridine. About 77% to 89% of the radioactivity was extracted from the soil using pyridine. The pyridine extracted soils were then combusted to attempt to obtain a mass balance for the ^{14}C-labeled compound. About 4% to 18% of the radioactivity was not extracted by pyridine. To see if there was any evidence of primary degradation of copoly VP/ST in these soils, samples of the pyridine extracts were analyzed using gel permeation chromatography and compared with polystyrene standards. Examination of the chromatographs showed no evidence of copoly VP/ST degradation in this study.[22]

From these data it is reasonable to conclude that, irrespective of the soil type, this polymer is very resistant to biodegradation and is not expected to biodegrade in the terrestrial environment.

d. Summary:

Fate of Styrene and 2-Vinylpyridine in the Environment

The 1.9 lb/year of each monomer that is estimated to enter the soil environment is expected to volatilize into the air. Assuming that the monomers are continuously released from a single point source, and utilizing a technique for approximating the impact of area sources[18], the predicted maximum ambient concentrations of styrene and 2-vinylpyridine are 57 ppt and 61 ppt respectively. This methodology predicts the highest possible concentration of monomers in ambient air.

Fate of Copoly VP/ST in the Environment

Copoly VP/ST is a stable polymeric substance not amenable to biodegradation, and therefore, is expected to remain in soils when disposed of to agricultural land as a component of animal excreta used as manure (fertilizer). Taking into account the very low aqueous solubility (88.6 to 185.6 ppb) of this polymer and the high potential to be absorbed by the soil (1.08×10^5), it is expected to have a low mobility through soil. It seems reasonable to assume that copoly VP/ST will not reach surface or ground waters from agricultural runoff from soils to which it has been disposed. As mentioned previously, this is a high molecular weight polymer and no loss due to volatization is expected. Based on its high molecular weight, low aqueous solubility, and lack of absorption by the rat, this polymer is not expected to bioaccumulate in plants or terrestrial organisms.

8. Environmental Effects of Released Substances

a. Talc

Talc is a naturally occurring hydrated magnesium silicate. Because of its inherent chemical stability, talc is used in the leather, rubber, textile, and machine construction industries. It is also used as a carrier for pesticides and in cosmetics and pharmaceutical, feed, and foodstuff formulation.[23] The general recognition of safety for use of talc in human dietary supplements was affirmed by FDA to an unidentified trade association.[24] Therefore it is judged to be safe for use in animal feed supplements.

b. 2-Vinylpyridine and Styrene

Environmental Effects:

Air:

There are no national ambient air standards for styrene and 2-vinylpyridine. In cases where national air standards are not available and a comparison number is needed for risk assessment, one approach is to start with a well accepted occupational health standard such as the American Conference of Industrial Hygienists Threshhold Limit Values (TLV's) and divide by appropriate safety factors. The safety factors are intended to account for the following differences:

1). Hours per week of exposure - 40 for workforce, 168 for the general population;
2). Years per lifetime of exposure - 50 for workforce, 100 for the general population;
3). Nature of the population - 18-65 years old and healthy for the workforce versus a variable group for the general population, including the young, the old and infirm;
4). The nature of the exposure - voluntary for the workforce versus involuntary for the general population;
5). The ability to observe effects - easier in the workforce, harder in the general population; and,
6). The size of the population - workforce smaller, general population larger.

Depending on the toxicity of the chemical being considered, different safety factors are used. For example, one ambient air guideline uses a factor of 300 for high and moderate toxicity contaminants and 50 for low toxicity contaminants.[25] In the referenced guideline, styrene is considered a moderate toxicity contaminant. Applying a safety factor of 300 to the 1986-7 TLV, an ambient air screening guideline of 50 ppm/300 = 0.12 ppm is obtained. The estimated air level of styrene from release of the monomer to the air for the above application using the worse case scenario is three orders of magnitude below the ambient air screening level.

In cases where a documented occupational health value does not exist, comparison to compounds of similar structure and toxicity for which an occupational value does exist is often used. No occupational health limit is available for 2-vinylpyridine. Using the TLV for pyridine, and using a safety factor of 300 for high toxicity contaminants, an ambient air screening guideline of 5 ppm/300 = 0.017 ppm or 17 ppb is derived. The estimated air level for 2-vinylpyridine from release of the monomer to the air for the above application using the worse case scenario is greater than two orders of magnitude below the ambient air screening level.

Water and Soil:

Summaries of the environmental effects of styrene and 2-vinylpyridine on aquatic life, waste treatment facilities, and plants are given in Tables 1 and 2. The data are taken from Eastman Kodak Company Environmental Safety Data Sheets which are in Appendices 5 and 6.

Table 1

Environmental Effects of Styrene
AQUATIC EFFECTS

Test Species	**Test** Duration	**LC50* Point** Estimate
Fathead Minnow *Pimephales promelas* (Pp)	96 hr	¦ 100 mL/L (Hard Water)
Fathead Minnow *Pimephales promelas* (Pp)	96 hr	46.4 mL/L (Soft Water)
Water Flea *Daphnia magna* (Dm)	96 hr	ï 100 mL/L
Sideswimmer *Gammarus fasciatus* (Gf)	96 hr	ï 100 mL/L
Snail *Helisoma trivolvis* (Ht)	96 hr	ï 100 mL/L
Bluegill Sunfish *Lepomis machrochirus* (Lm)	96 hr	25.1 mL/L (Soft Water)
Goldfish *Carassius auratus* (Ca)	96 hr	64.7 mL/L (Soft Water)

*LC50 = Lethal Concentration to 50% of the population.

SECONDARY WASTE TREATMENT COMPATIBILITY

5-hr IC50* = ï 5000 mL/L

*IC50 = The concentration of chemical that inhibits, by 50%, glucose metabolism by secondary waste treatment microorganisms.

PLANT GROWTH EFFECTS

GERMINATION	Test Duration	No Observed Effect Concentration (adverse)
Ryegrass (*Lolium perenne*)	7 Days	100 mL/L
Radish (*Raphanus sativus*)	7 Days	100 mL/L
Lettuce (*Lactuca sativa*)	7 Days	100 mL/L

Table 2.

Environmental Effects of 2-Vinylpyridine
AQUATIC EFFECTS

Test Concentration Species	Test Duration	LC50* Point Estimate and (95% Confidence Limits)	No Observed Effect (Acute)
Fathead Minnow <u>Pimephales</u> <u>promelas</u> (Pp)	96 hr	4.0 mL/L (1-10 mL/L)	1.0 mL/L
Water Flea <u>Daphnia</u> <u>magna</u> (Dm)	96 hr	3.2 mL/L (1-10 mL/L)	1.0 mL/L
Sideswimmer <u>Gammarus</u> <u>fasciatus</u> (Gf)	96 hr	3.2 mL/L (1-10 mL/L)	1.0 mL/L
Flatworm <u>Dugesia</u> <u>tigrina</u> (Dt)	96 hr	3.2 mL/L (1-10 mL/L)	1.0 mL/L
Snail <u>Helisoma</u> <u>trivolvis</u> (Ht)	96 hr	3.2 mL/L (1-10 mL/L)	1.0 mL/L
Segmented Worm <u>Lumbriculus</u> <u>variegatus</u> (Lv)	96 hr	32 mL/L (10-100 mL/L)	10.0 mL/L
Pillbug <u>Asellus</u> <u>intermedius</u> (Ai)	96 hr	3.2 mL/L (1-10 mL/L)	1.0 mL/L

*LC50 = Lethal Concentration to 50% of the population.
Point Estimate Calculated By: Non-Linear Interpolation.

SECONDARY WASTE TREATMENT COMPATIBILITY

5-hr IC50* = 1200 mL/L

*IC50 = The concentration of chemical that inhibits, by 50%, glucose metabolism by secondary waste treatment microorganisms.

PLANT GROWTH EFFECTS

GERMINATION	Test Duration	No Observed Effect Concentration (adverse)
Ryegrass (<u>Lolium</u> <u>perenne</u>)	7 Days	10 mL/L
Radish (<u>Raphanus</u> <u>sativus</u>)	7 Days	10 mL/L
Lettuce (<u>Lactuca</u> <u>sativa</u>)	7 Days	10 mL/L

Human Health Effects:

The monomers, styrene and 2-vinylpyridine, have respectively moderate and fairly high acute toxicities and are both moderately toxic on subchronic administration to animals. Eastman Kodak Company and its production affiliates maintain extensive environmental controls to eliminate unnecessary exposure of employees to chemical substances. As a result of these controls, exposure of employees to the monomers, 2-vinylpyridine and styrene, at the manufacturing site are expected to be quite low. When the commercial process is implemented, it will be monitored by Eastman Chemicals Division's industrial hygiene staff to ensure that worker exposure is indeed adequately low. In the case of styrene, limits have been set by OSHA at 100 ppm, 8-hr TWA; 200 ppm acceptable ceiling; and 600 ppm maximum ceiling (5 min in 3 hr). NIOSH recommendations for styrene are: 50 ppm (213 mg/m^3) TWA; 100 ppm ceiling. Health effects considered were eye and respiratory system irritation and nervous system effects. NIOSH comments on styrene: action level should be set at 25 ppm; skin contact is to be prevented; and workers should be warned of possible adverse reproductive effects.[26]

2-Vinylpyridine(2-VP):[27]

Acute and Short-Term Studies.[27] Toxicity studies in animals from the Laboratory of Industrial Medicine, Eastman Kodak Company, and the Russian literature show 2-VP to be fairly acutely toxic and to be readily absorbed through the skin following contact with the liquid or vapor. More extensive acute studies and a 14-day gavage study in rats were performed by the Toxicology Section, Health and Environment Laboratories, Eastman Kodak Company. The oral LD_{50} of 2-VP was 336 mg/kg for male and female rats when the neat compound was intubated, but when gavaged as a 20% suspension in corn oil the LD_{50} was 951 mg/kg in fasted and fed male rats, 673 mg/kg in fasted female rats, and 951 mg/kg in fed female rats. The 2-VP was a strong eye irritant to rabbits and a strong irritant and sensitizer for guinea pig skin. The dermal LD_{50} on guinea pigs was 0.16 mL/kg.[27]

Subchronic Study.[28] A 90-day subchronic gavage study in which rats were dosed by gavage with suspensions of 2-VP in corn oil was performed by Toxicology Section, Health and Environment Laboratories, Eastman Kodak Company. Doses were 0, 20, 60, and 180 mg/kg per day, 5 days per week, for 13 weeks. Systemic effects at the high dose included: reduced body weight gain in male rats; reduced feed consumption in male rats, and, toward the end of the study, increased feed consumption in female rats; a slight increase in number of platelets in both sexes; a slight increase in aspartate amino transferase (AAT) in male rats; increased or decreased absolute organ weights of brain, heart, and adrenal glands, and relative to body weight, organ weights of liver, kidneys, brain, adrenal glands, and testes of male rats; abnormal absolute organ weights of liver and relative weights of liver, kidneys, and ovaries in females. The middle dose produced increased AAT in male rats, increased relative liver to body weight ratios in both sexes, and increased relative liver to brain weights in female rats.

The higher doses of 60 to 180 mg/kg also produced local effects due to irritation of the gastric mucosa. These involved primarily the nonglandular epithelium and were characterized by degeneration of the superficial epithelial cells at the highest dose, and at both of the higher doses, hyperkeratosis and acanthosis of the epithelium resulting in thickening of the nonglandular epithelium and mild inflammatory changes (congestion, edema, and inflammatory cell infiltration). No other remarkable gross or microscopic pathology was observed at any dose.

The lowest dose of 20 mg/kg did not produce any significant local or systemic changes in either sex.[27,28]

Short-Term In Vitro Tests. The 2-VP was negative in three in vitro short-term predictive tests: Salmonella rat-liver microsome reverse mutation (Ames) test, Chinese hamster ovary HGPRT forward-mutation test, and unscheduled DNA incorporation test. Thus, 2-VP appears not be genotoxic.[27,29]

Styrene[30]

An extensive review of the toxic effects of styrene in man and animals and an evaluation of these effects with regard to setting worker protection standards has been published by the U.S. National Institute of Occupational Safety and Health.[31]

Acute Toxic Effects. Styrene is readily absorbed through the lungs of man and animals from the gaseous phase and, less rapidly, through the skin from the gaseous and liquid phases. Absorbed styrene is readily detoxified and eliminated, partially through the lungs, but mainly through the elimination of metabolites in the urine. The acute oral LD_{50} of styrene is reported to be 5000 mg/kg in rats and 360 mg/kg in mice. Acute exposure to the liquid or vapor produces mainly irritation of the skin, eyes, and respiratory tract. It affects the central nervous system of animals and man and produces in humans, following prolonged exposures to high levels, neurological disturbances, but has no acute effect on the hematopoietic system of animals.

Subchronic and Long-Term Studies. In a series of whole-body exposure studies, guinea pigs exposed to styrene were susceptible to acute lung infiltration and death at vapor levels that had no effect on rats, rabbits, or dogs. No significant changes were found on gross and microscopic pathology in any animals. Oral intubation of 667 mg/kg of styrene per day in rats produced slight effects on growth and organ weights; 133 mg/kg was a NOEL. Rats exposed to 300 ppm styrene vapor for 11 weeks had liver alterations. Rats dosed in drinking water with 7.7 and 14 mg/kg (males) or 12 and 21 mg/kg (females) of styrene for 2 years showed no significant differences from controls in any physiological value measured, in clinical signs, or in incidences of tumors or other lesions found on gross or microscopic pathology (Litton).

In dogs, styrene intubated at levels of 400 or 600 mg/kg per day for up to 561 days produced consistent changes in the formed blood elements that were readily reversible when administration of styrene was stopped; 200 ppm was a NOEL. No significant toxicity was seen on gross or microscopic pathology.

Effects on the liver and hematological and pulmonary systems and on the central nervous system have been reported in humans exposed to styrene for extended periods. It is not possible to relate these findings to dose.

Reproductive Effects. Several studies in rats by whole-body exposure at 12 or 47 ppm styrene vapor or by gavage at 90 or 150 mg/kg twice a day indicate that styrene is not embryotoxic, fetotoxic, or teratogenic in rats at levels that are toxic to the dams. Rats and rabbits exposed by whole-body exposure to 300 and 600 ppm styrene vapor showed no embryotoxic, fetotoxic, or teratogenic effects. Pregnant mice exposed to 250 to 1000 ppm of styrene vapor showed increased embryolethality and terata at doses that were toxic to the dams. Hamsters exposed to 750 ppm styrene showed no significant effect on fetuses, whereas at 1000 ppm there were embryolethal effects, but no malformations were found.

Epidemiological studies in humans have given conflicting results, and in many studies confounding factors could not be properly controlled. Several studies, however, have suggested that styrene may adversely affect reproductive success, evidenced as spontaneous abortions in females occupationally exposed to high levels of styrene.

Mutagenic and Clastogenic Effects. Styrene has produced extremely irregular results in *in vitro* short-term predictive tests. Similar uneven results have been found in experiments in animals and in studies of humans occupationally exposed to styrene. Taken together, the results suggest that styrene is a weak mutagen and clastogen.

Carcinogenesis. Styrene has been studied for oncogenic effects in 8 recent and more or less adequate studies as follows: In rats by inhalation at 600 and 1000 ppm of styrene (Dow); by gavage in olive oil in 2 strains of mice and 1 strain of rats (IARC); a mixture of styrene and beta-nitrostyrene by gavage in rats and mice (NTP); and styrene by gavage in rats and mice (NTP). In the Dow study, while neither male nor female rats showed a significant increase in tumors of any site, female rats had nonsignificant increases in the combined frequencies of lymphoid and hematopoietic system tumors. In the IARC studies, which were complicated by deaths due to surpassing the MTD, one strain of mice showed a significant increase in liver tumors in females and a nonsignificant increase in males, whereas the other mouse strain and the rats showed only nonsignificant increases in tumor incidence at a few livers sites.

Styrene caused significant toxic lesions of the liver in the first mouse study. In the bioassay of a mixture of styrene and beta-nitrostyrene, NTP concluded that there was no convincing evidence that the mixture was carcinogenic in rats or in mice. In the NTP gavage study of styrene, there was a significant positive association between styrene dose and incidence of combined adenomas and carcinomas of the lung of male mice compared to the contemporary control rats. The variation of incidence of these neoplasms in historical control mice in the laboratory during the tests, however, precluded a firm conclusion of carcinogenicity at that site. There were no other significant differences in tumor rates among either species or sex. In addition, no excess tumors were found in the Litton 2-year drinking-water study referred to above.

Epidemiological studies of workers occupationally exposed to styrene have always shown a decrease in total deaths and total deaths from cancer compared to the general population (healthy worker phenomenon). This is also true for site-specific cancer incidence except for 2 studies showing an increase in leukemias. The workers in these 2 studies may have been exposed to benzene or other solvents.

In addressing the question of carcinogenicity, NIOSH comments (p. 128), "From the experimental animal investigations and from the epidemiological studies, there seems little basis to conclude that styrene is carcinogenic." They comment further, "If styrene oxide is an intermediate metabolite, convalent binding to nucleic acids leading to cancer development might be predicted; however, there is little evidence that this epoxide is formed in vivo. Nonetheless, the enzyme catalyzing the formation of this epoxide from carbon-carbon double bonds exists in many tissues, as do the enzymes catalyzing the hydration or other inactivation of the epoxide." And conclude, "Thus, while it does not seem appropriate from presently available evidence to conclude that styrene can cause cancer among exposed workers, there is enough evidence to suggest that it might be at least a weak carcinogen, and priority should be given to further studies of this problem."[30] There has been no recent evidence that would change this position.

Conclusion

The calculated maximum annual release of 2-vinylpyridine and styrene to the environment is 1.9 lb of each. This is approximately 0.24 ppt of each in soil, much less in water and 60 ppt in air, if they are transferred completely to these compartments. The data in Tables 1 and 2 for soil and water and the threshold limit value arguments for air indicate that these monomers will have virtually no effect on the environment at the maximum use levels. In addition, the mammalian toxicity of these two monomers discussed above is similarly very low compared to the maximum expected concentrations. Therefore, it is concluded that no environmental effects are likely to result from either of these monomers.

c. Copoly VP/ST

Environmental Effects:

The petitioner has examined the effects of copoly VP/ST on plant seedlings, secondary waste treatment microorganisms, and earthworms.

Plant Seedling Effects

A study was performed to determine the maximum concentration of copoly VP/ST which has no effect on the germination and early growth of corn, lettuce, marigold, radish, and soybean.[32] No significant adverse effects were detected at the highest level tested, 1000 mg of copoly VP/ST per kg of soil, 1000x the maximum annual exposure level. However, statistically significant dose-related decreasing trends in corn and soybean height and lettuce root length were observed in this test.

Therefore, a more definitive plant growth study for corn, soybean, and lettuce was performed. This study, conducted in accordance with FDA Technical Assistance Document 4.07, March 1987, employed 10 replicates of 5 seedlings each, exposed to 0, 50, 100, 200, 500 and 1000 mg of copoly VP/ST per kg of quartz sand. Shoot height, shoot weight, and root weight were measured.[33]

For shoot height and shoot weight, no significant differences were detected for any of the three plant species. The No Observed Effect Concentration (NOEC) was determined to be 1000 mg/kg for each of these two variables.

Corn and lettuce root weights were greater than controls at higher doses so the NOEC was 200 mg/kg. For soybean the NOEC was 1000 mg/kg. No adverse effects were observed, even at 1000 mg/kg.

For percent elongation, the NOEC for lettuce and soybean was 1000 mg/kg. For corn, elongation was observed at the highest level so the NOEC for corn elongation was 500 mg/kg.

As described on page 13 of this assessment, the expected amount of copoly VP/ST per year is approximately 1 mg/kg of soil. All of the NOEC's for adverse effects were 1000 mg/kg except for corn elongation at 500 mg/kg. With no polymer degradation it would be 500-1000 years before any effect might occur. Accordingly, it is very unlikely that this polymer, entering the environment at the rate of 1 mg/kg of soil, will have any effect on plant growth.

Secondary Waste Treatment Compatibility

A radiorespirometric method was used to determine the compatibility of copoly VP/ST with secondary waste treatment microorganisms.[34] In this study, sludge microorganisms efficient in metabolizing glucose were exposed to several concentrations of copoly VP/ST, the highest of which did not exceed 1/4 of its limiting aqueous solubility.

The ratios of the % conversions of D-(U-^{14}C)glucose to $^{14}CO_2$ in the presence of various levels of copoly VP/ST to the % conversion of D-(U-^{14}C)glucose to $^{14}CO_2$ in the absence of copoly VP/ST were used to define a dose-response relationship. Potassium dichromate was used as the positive control.

To each of 27 respirometer flasks was added 5.0 mL of activated sludge solution that contained 10 mg of sludge solids per mL. Four groups of flasks (three replicates per group) then received varying amounts of copoly VP/ST. Another four groups of flasks (three replicates per group) received varying amounts of dichromate. The remaining 3 flasks received 2.5 mL of 0.02 M phosphate buffer (negative control). Each of the 27 flasks then received 2.5 mL of a D-(U-^{14}C)glucose solution (approximately 0.3 mCi). The resulting copoly VP/ST concentrations were 24 mg/L, 2.4 mg/L, 0.24 mg/L, and 0.024 mg/L. The dichromate (positive control) exposure concentrations were 333 mg/L, 167 mg/L, 33 mg/L, and 3.3 mg/L. The flasks were sealed with clean serum stoppers and incubated in the dark at 27°C in a reciprocating incubator-shaker for 5 hours. At the end of the incubation period the contents of each respirometer flask were acidified. The $^{14}CO_2$ absorbing vials were detached from the respirometers and the trapped $^{14}CO_2$ assayed in a scintillation spectrometer.

In the negative control samples (without copoly VP/ST or dichromate), 31.46% of the D-(U-^{14}C)glucose was metabolized to $^{14}CO_2$. The minimum acceptable value is 15%. The microorganisms showed a concentration-related effect to the positive control (dichromate); this was expected. Copoly VP/ST at all concentrations tested had no effect on glucose metabolism by the microorganisms.[34]

Copoly VP/ST would not be expected to affect secondary waste treatment microorganisms adversely as a result of exposure to concentrations <24 mg/L. This concentration is approximately one-fourth the limiting aqueous solubility of this polymer at pH values similar to those in most soils and surface waters.

<u>Earthworm Toxicity Study</u>[35]

The petitioner contracted this study to Biospherics Incorporated, Rockville, Maryland. The purpose of the study was to determine the dose-response relationships of copoly VP/ST effects upon earthworms (dungworms).

Dungworms (<u>Eisenia</u> <u>foetida</u>) were kept under relatively controlled laboratory conditions and were exposed to soil concentrations of copoly VP/ST of 0, 62.5, 125, 250, 500, or 1,000 mg polymer/kg soil for a 28-day period. Lethal and sublethal effects of copoly VP/ST on this species of earthworm were monitored on days 7, 14, and 28. Significant procedural difficulties in this test prevented a definitive result from being determined; however, it appears accurate to conclude that the following preliminary statements about the toxicity of copoly VP/ST to earthworms can be made.

Mortality in dungworms exposed to graded doses of copoly VP/ST was seen at almost all treatment and control levels at days 7, 14, and 28. The mortality ranged from 0% in the 250 mg/kg dose group to 10% in the 1,000 mg/kg dose group, with 5% mortality in the control group. An LC_{50} could not be determined from this experiment, but the LC_{50} appeared to be ¦1,000 mg polymer/kg soil. Sublethal effects (soft, soft and flaccid, and moribund) were also monitored. An interpretative description of "soft" and "soft and flaccid" are: "soft" - less muscle tone, but the activity is equivalent to that of a normal worm; and, "soft and flaccid" - soft muscle tone with decreased mucus production and impaired movement when stimulated by prodding. Significant sublethal effects were evident in all treatment groups by either 7 or 14 days, and became progressively more severe throughout the 28-day experiment. The sublethal characteristic "soft" was observed among all treatments, but "soft and flaccid" was only observed at 250 mg/kg, 500 mg/kg, and 1000 mg/kg, and then only on day 28.[33] "Moribund" effects were not observed in this study.

Human Health Effects

Except for mutagenicity testing, copoly VP/ST has not been tested for toxicity. However, a polymer having virtually the same molecular weight distribution and chemical and physical properties but prepared from 2-methyl-5-vinylpyridine (2M5VP) has been tested.

Poly(2-methyl-5-vinylpyridine-co-styrene) (copoly 2M5VP/ST) was at most only slightly toxic when given in a single oral dose to rats or mice, having an acute oral LD_{50} in excess of 3200 mg/kg in each species. When applied to the skin of guinea pigs under an occlusive wrap for 24 hours, it caused only slight edema and some desquamation. No evidence of absorption was apparent. Copoly 2M5VP/ST failed to sensitize any of ten guinea pigs treated. Repeated skin application (ten days) caused only slight and spotty erythema on the five guinea pigs tested. When applied to the eye of rabbits the compound caused slight erythema. Copoly 2M5VP/ST was fed to rats and dogs at up to 5% in the diet for 90 days. There were no effects in either species except for those attributable to decreased feed intake or substitution of a nonnutritive material for part of the diet in high dose rats. Copoly 2M5VP/ST, labeled with carbon-14, was not shown to be absorbed from the gastrointestinal tract of rats. The Center for Veterinary Medicine has agreed that the results of the tests could be extrapolated to the present polymer, copoly VP/ST. Copoly VP/ST was not a mutagen in the standard plate-incorporation salmonella reverse-mutation assay, with and without rat-liver microsomes.

These studies demonstrate that Copoly VP/ST has very low acute and chronic toxicities in experimental animals and is not absorbed from the gastrointestinal tract. Thus, the polymer is not expected to cause adverse effects to humans during its manufacture, use, or disposal.

d. Summary

Styrene and 2-vinylpyridine are expected to be released in very low amounts (<2 lb per year, nationwide) and the toxicity to aquatic and terrestrial organisms is low compared with the expected concentrations (0.24 parts per trillion in soil and less than this value in air and water). Therefore, it is concluded that these two monomers will have virtually no effect on the environment.

Talc is a natural product that is generally accepted as safe for a wide variety of uses in foods and medicinals.

It is assumed that the fatty acids and amino acids are metabolized by beef animals and do not reach the environment.

Copoly VP/ST will not have a significant adverse effect on microorganisms or plants at <1000 mg/kg of soil. Significant lethal effects were not observed on earthworms even at the highest level tested, 1000 mg/kg. Responses of worms demonstrated less muscle tone, but with the activity of normal worms, even at the lowest level tested, 62.5 mg/kg. However, at the proposed use levels, disposal of 1.17 mg Copoly VP/ST/kg of soil/year to the environment is not expected to have any adverse effects.

9. Utilization of Natural Resources and Energy

a. Production

Approximately 31.6 pounds of low-pressure steam, 0.38 kw of electricity, and 0.12 ton-hours of refrigeration will be used to produce one pound of copoly VP/ST. All these utilities are generated from coal-fired power plants. The active ingredients in the polymer, 2-vinylpyridine and styrene, are purchased materials which the petitioner understands are derived from by-products of the petroleum industry.

b. Transport

The shipping of this material between plants during manufacture and to users will require petroleum as fuel.

c. Use

The incorporation of the RPAA into cattle feed is not expected to require any additional energy. The use of electricity or fuel during the feeding of cattle is not expected to require more than would normally be used.

d. Disposal

The polymer portion of the RPAA will be disposed of to the terrestrial environment in the manure (fertilizer). The presence of copoly VP/ST will not require any additional energy requirements.

Wastes from the production of copoly VP/ST, if any, will be disposed of in petitioner's extensive waste treatment facilities with no significant effects on the environment.

e. Effects Upon Endangered Species or Historic Places

The petitioner has demonstrated that copoly VP/ST, when used as intended, will not adversely affect plants or animals. Likewise, the disposal of feces containing copoly VP/ST to land is not expected to have any effect on any place or structure identified in the National Register of Historical Places.

f. Disruption of the Physical Environment from the Production of Copoly VP/ST, Use in the Manufacture of RPAA, and Disposition as a Feed Additive to Ruminant Animals

Production of copoly VP/ST and RPAA is through established processes familiar to and used by petitioner's affiliates, Tennessee Eastman Company and Arkansas Eastman Company, for products other than copoly VP/ST and is expected to have no effect on the local physical environment. Certainly the incorporation of RPAA as produced by Eastman in the diets of ruminant animals will have no detectable effect on that environment.

10. Mitigation of Potential Adverse Environmental Effects

The petitioner's control of volatile organic chemical emissions in its manufacturing facilities and treatment of effluents in its waste treatment facilities reduce to a minimum emissions and effluents that have the potential for adverse effects. Because of the efficiency of air and water treatment facilities in the manufacture of copoly VP/ST and the production of RPAA, only insignificant quantities of any potential environmentally adverse materials are likely to be disposed of to the aquatic, atmospheric, or terrestrial environments.

Disposal to the terrestrial environment of talc at a maximum annual rate of 4.4 mg/kg of soil and copoly VP/ST at a maximum annual rate of 1.17 mg/kg as a result of feeding RPAA are not expected to adversely effect plants and animals. Copoly VP/ST has been shown to be resistant to biodegradation in soil and in secondary waste treatment systems; however, is not expected to bioconcentrate in soil or aquatic organisms. Therefore, the environment is not expected to be affected adversely by this proposed use of copoly VP/ST.

11. Alternatives to the Proposed Action

a. Alternatives

As no potential adverse effects have been identified resulting from the proposed action, the petitioner concludes that it is unnecessary to suggest alternative actions.

b. Environmental Benefits of the Proposed Action

It is anticipated that the use of RPAA will increase the efficiency of meat production through more effective use of cattle feed. This increased efficiency of food consumption could lead to more productive use of the land for raising grain and other agricultural products.

c. Environmental Risks of the Proposed Action

The polymer is not expected to have any adverse effects on wildlife or soil organisms at the concentrations expected to be disposed of to the terrestrial environment (1.17 mg copoly VP/ST per kg soil/year). It is expected to be inert in soil, existing in a finely divided state. The polymer is not expected to affect earthworms, other soil organisms, or plants at anticipated disposal concentrations. The polymer does not have sufficient volatility to present a hazard to the atmosphere. With a limiting solubility of about 90-180 ppb in water, this polymer will not pose a hazard to the aquatic environment.

12. List of Preparers of the Environmental Assessment

Person	Area of Responsibility
Mr. G. T. Luce Material Safety Program Eastman Chemicals Division Eastman Kodak Company Kingsport, Tennessee	Regulatory Affairs (TSCA, EPA, FDA)
Mr. J. W. Gorsuch Health and Environment Laboratories Eastman Kodak Company Rochester, New York	Environmental Fate and Effects
Dr. E. G. Miller Material Safety Program Eastman Chemicals Division Eastman Kodak Company Kingsport, Tennessee	Regulatory Affairs (FDA)

Person	Area of Responsibility
Mr. Peter Morison Material Safety Program Eastman Chemicals Division Eastman Kodak Company Kingsport, Tennessee	Regulatory Affairs (FDA)
Mr. R. C. Reynolds Health and Environment Laboratories Eastman Kodak Company Rochester, New York	Product Safety and Toxicology
Dr. Kenneth A. Robillard Health and Environment Laboratories Eastman Kodak Company Rochester, New York	Environmental Fate and Effects

13. Certification

The undersigned official certifies that the information presented is true, accurate, and complete to the best of the knowledge of Eastman Chemical Company, Eastman Kodak Company.

Robert E. Keith

Robert E. Keith, M.D.
Director
Product Safety and Environmental Affairs

14. References

1. Food Additive Petition 2197, Heading H, Enclosure 6, Part A.
2. Ibid., Part B.
3. CHEMEST: A Program for Chemical Estimation, W. J. Lyman and R. J. Potts, (Editors), Arthur D. Little, Inc., 1985.
4. Eastman Chemicals Division Research Laboratories data, L. A. Cook, 1986.
5. Whittaker, Clark Daniels, Inc., Material Safety Data Sheet, 1984.
6. The Merck Index, Merck & Co. Inc., Rahway, N.J., 1983, p. 1259.
7. Ibid., p. 858.
8. Ibid., p. 806.
9. Handbook of Environmental Data on Organic Chemicals, K. Verschueren, Van Nostrand Reinhold Co., New York, N.Y., 1983, pp. 1055-1056.
10. Reilly Tar and Chemical Corp., Material Safety Data Sheet, 1985.
11. Priv. Comm., Steve Noyes, National AG Statistics Service, USDA, 1990.
12. Eastman Chemicals Division Research Laboratories data, L. E. Deetz, 1985.
13. Food Additive Petition 2197, Heading H, Enclosure 1.
14. Ibid., Enclosure 2.
15. Priv. Comm., Charles Strasia, Oklahoma State University Extension Center, to L. E. Deetz, Eastman Kodak Company, 1986.

16. The Feedlot, I. A. Dyer and C. C. Mary, Lea & Febiger, Philadelphia, 1972, pp. 172-173.
17. U.S. FDA, from Sample Environmental Impact Analysis Report provided to Eastman Kodak Company, July 5, 1984.
18. Turner, D.B., Workbook on Atmospheric Dispersion Estimates, EPA Office of Air Programs, P. AP-26. Research Triangle Park, N.C., 1970.
19. C. Tagesson, P. A. Andersson, T. Andersson, T. Bolin, M. Kallberg, and R. Sjodahl, Scand. J. Gastroenterology, 18, 481, (1983).
20. Food Additive Petition 2197, Heading E, Enclosure 15.
21. Ibid., Heading H, Enclosure 6, Part D.
22. Ibid., Part C.
23. Ibid., Heading H, Enclosure 5.
24. Ibid., Enclosure 3.
25. New York State Air Guide -1, Guidelines for the Control of Toxic Contaminants, New York State/Department of Environmental Conservation, Division of Air Resources, 1985-6.
26. "NIOSH Recommendations for Occupational Safety and Health Standards", supplement to Morbidity and Mortality Weekly Reports, July 19, 1985, 34, No. 1S, p-26S, HHS Publication No. (CDC) 85-8017, Atlanta, GA.
27. Food Additive Petition 2197, Heading E, Enclosure 4.
28. Ibid., Enclosure 5.
29. Ibid., Enclosures 7,8 and 9.
30. Ibid., Enclosure 3.
31. National Institute for Occupational Safety and Health Criteria for a Recommended Standard: Occupational Exposure to Styrene, U.S. Department of Health and Human Services, Public Health Service, Center for Disease Control, DHHS (NIOSH) Publication No. 83-119, 250pp.
32. Food Additive Petition 2197, Heading H, Enclosure 6, Part E-1
33. Ibid., Part E-2.
34. Ibid., Part F.
35. Ibid., Part G.

15. Appendices

Appendix 1.

Descriptions of Procedures Used to Determine Physical/Chemical Estimates For Copoly VP/ST

I. CHEMEST Software

A. Introduction

The following estimates - boiling point, melting point, vapor pressure and soil adsorption coefficient - were obtained through the use of CHEMEST software. CHEMEST is an interactive computer system that provides estimates of environmentally important properties of organic chemicals. The procedures within CHEMEST are based on an estimation methods handbook[(1)] developed by Arthur D. Little, Inc. CHEMEST is available through online services of Technical Database Services, Inc.[(2)]

The estimation methods are limited as they are not designed for polymeric materials. The physical/chemical values can be approximated by considering a subunit of the polymer. For copoly VP/ST, an oligomer of 10 monomeric units was chosen. Every CHEMEST output provides information on the method error and, if appropriate, the propagated and total error. Method error for a given estimation method is the error that results when all inputs are accurately known. Propagated error is the additional error in the estimate due to the uncertainty in one or more of the inputs which may be estimated values. Total error is a combination of method and propagated error. It is calculated by CHEMEST whenever one or more of the inputs is an estimate with some non-zero. For additional information on the reported errors see reference (2), Chapter 3.2.7.

B. Vapor Pressure Estimation

The modified Watson method was used to estimate the vapor pressure of the oligomer. The method uses the following equation:

$$W H_v \quad Z \; W H_{vb} \; (3 - 2\,(T/T_b))^m$$

where:

- $W H_{vb}$ = heat of vaporization
- T = temperature of calculation
- T_b = boiling point
- m = constant, calculated from (T/T_b) ratio by CHEMEST

The heat of vaporization is calculated by CHEMEST using two parameters (a and b) which are associated with the polarity of the compound. The parameters are determined by choosing the compound class that best represents the polarity of the compound.

The input parameters for the estimation of the vapor pressure for the oligomer included:

Normal Boiling Point	$1000.1^{0}C$ (Estimated)
Melting Point	$574.4^{0}C$ (Estimated)
Identification of Physical State	Solid
Identification of Compound Class	Nonpolar or Slightly Polar Compounds (a = 1.50, b = 0.10)
Temperature of Calculation	$25.0^{0}C$

Since measured boiling point and melting point values were not available for the oligomer, estimates for both of these properties were obtained through CHEMEST. The boiling point was estimated using calculated values for molar refraction and parachor and a correcting parameter for chemical type. CHEMEST determines the molar refraction and parachor by summing fragment values for each atom, multiple bond and/or substructure in the compound. The melting point was estimated using the boiling point as the input parameter.

The estimated vapor pressure for the oligomer was 1.94×10^{-26} mm-Hg with a total error factor of 160.2. The breakdown of this total error factor is as follows:

Method Error:	x 10.0
Propagated Error:	x 92.2
T_b Component:	x 50.8
T_m Component:	x 9.4
Total Error:	x 160.2

CHEMEST calculated a value for vapor pressure but stated a warning message that the value was outside the accuracy range of the method. It can be assumed that the vapor pressure for the polymer would be less than or equal to that for the oligomer.
References: (1), Ch. 14 and (2), Ch. 4-6.

C. Soil Adsorption Coefficient
The soil adsorption coefficient for the oligomer was estimated from the water solubility. The procedure in CHEMEST uses several regression equations which vary by the chemical classes represented.

The following equation was chosen for copoly VP/ST based on the chemical class and low error associated with the correlation:
$\log K_{oc} = -0.54 \log S + 0.44$, where S = water solubility (mole fraction).

The chemical classes represented include mostly aromatics or polynuclear aromatics. The input parameter for the estimation was the measured water solubility values for the polymer, 0.18 mg/L at pH 9 (Health and Environment Laboratories Data).(3) The estimated soil adsorption coefficient for the polymer was 1.08×10^{5} with a total error factor of 2.0.
Reference: (1), Ch. 4.

II. References

1. Handbook of Chemical Property Estimation Methods, W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, (Eds.), McGraw-Hill Book Co., 1982.

2. CHEMEST: A Program for Chemical Estimation, W.J. Lyman and R.J. Potts, (Eds.), Arthur D. Little, Inc., 1985.

3. Ziegler, D.A., Specific Buffer Solubility - Poly(2-vinylpyridine-co-styrene) (copoly VP/ST), Health and Environment Laboratories, Report #ETS-TR84-57, 1984.

Appendix 2.

Description of Procedures Used to Determine Physical/Chemical Estimates for Styrene

I. MedChem Software

A. Introduction

The estimate for the octanol/water partition coefficient (K_{ow}) was obtained through the use of Pomona MedChem Software, Release 3.33.[1] The software is based on a procedure which assigns fragment constants to structural subunits. The calculated log K_{ow} is the sum of fragment constants appropriate for the molecule in question.[2] These calculations have been developed into a computer algorithm called CLOGP.[3] The software is a commercially available package from Pomona College.

B. Input Parameter

A chemical nomenclature system, called SMILES, is used to enter the chemical structure as input for the CLOGP algorithm. A SMILES specification uniquely describes the hydrogen suppressed graph of a chemical structure in a way that also defines hydrogen attachments and bond types. More information on SMILES can be obtained from the MedChem Software Manual, Release 3.33. The SMILES input for styrene was:

c1cccc(C=C)c1

C. Results

Four types of structural subunits and bonds were defined for the styrene molecule and are listed with their corresponding fragment values in the following table.

Class	Type	Log (P) Contribution Description	Value
Isolating	Carbon	2 Aliphatic isolating carbon(s)	0.390
Isolating	Carbon	6 Aromatic isolating carbon(s)	0.780
Exfragment	Hydrogen	8 Hydrogen(s) on isolating carbons	1.816
Exfragment	Bonds	1 Chain and 0 alicyclic (net)	-0.120

The CLOGP algorithm calculated the log K_{ow} value at 2.866. No error level was determined as all fragment constants were measured values.

II. CHEMEST Software

A. Introduction

The following estimates for styrene - boiling point, melting point, vapor pressure, Henry's Law Constant, volatilization from water, water solubility, soil adsorption coefficient and bioconcentration factor - were obtained through use of CHEMEST software. CHEMEST is an interactive computer system that provides estimates of environmentally important properties of organic chemicals. The procedures within CHEMEST are based on an estimation methods handbook[4] developed by Arthur D. Little, Inc. CHEMEST is available through online services of Technical Database Services, Inc.[5]

Every CHEMEST output provides information on the method error and, if appropriate, the propagated and total error. Method error, for a given estimation method, is the error that results when all inputs are accurately known. Propagated error is the additional error in the estimate due to the uncertainty in one or more of the inputs which may be estimated values. Total error is a combination of method and propagated error. It is calculated by CHEMEST whenever one or more of the inputs is an estimate with some non-zero. For additional information on the reported errors see reference (5), Chapter 3.2.7.

B. Boiling Point

The Meissner method was used to estimate the normal boiling point of styrene. It is based on correlating the boiling point with molar refraction (R_D), parachor (P), and a parameter for chemical type (B):

$$T_b = \frac{637\ (R_D)^{1.47} + B}{(P)}$$

where; T_b = boiling point
R_D = molar refraction
P = parachor
B = constant whose value depends on chemical type

CHEMEST calculates R_D using the atomic refraction contribution method of Eisenlohr which consists of summing contributions for each atom, multiple bond and/or substructure in the compound. Parachor is calculated using a similar contribution scheme. The input values for R_D and P were obtained from Table 12-3 and follow:

Molecular Feature	Number	R_D	P
Benzyl	1	25.207	190.0
-C=C-	1	6.569	37.4

Calculated values for R_D and P were 31.8 and 227, respectively. The parameter B is used to adjust the computation of boiling point for compound type. The input value for B was obtained from Table 12-5:

B = -2500 (aromatic hydrocarbon)

The R_D, P, and B were input into the above equation to calculate an estimated boiling point of 168 ^{0}C with 5.0% total error.

Reference: (4), Ch. 12.

C. Melting Point

The following equation was used to estimate the melting point of styrene in the CHEMEST software:

$T_m = 0.5839\ T_b$

where: T_m = melting point
T_b = boiling point

The input parameter was the measured boiling point, 145^{0}C. The estimated melting point was calculated at 5.2^{0}C with 8.4% total error.

Reference (5), Ch. 4-9.

D. Vapor Pressure Estimation

The modified Watson method was used to estimate the vapor pressure of styrene. The method uses the following equation:

$W H_v \ Z \ W H_{vb}\ (3 - 2\ (T/T_b))^m$

where: $W H_{vb}$ = heat of vaporization
T = temperature of calculation
T_b = boiling point
m = constant, calculated from T/T_b ratio by CHEMEST
(m = 0.19 for liquids)

The heat of vaporization is calculated by CHEMEST using two parameters (a and b) which are associated with the polarity of the compound. The parameters are determined by choosing the compound class that best represents the polarity of the compound.

The input parameter for the estimation of the vapor pressure of styrene included:

Normal Boiling Point	145^0C (measured)
Identification of Physical State	Liquid
Identification of Compound Class	Nonpolar or Slightly Polar Compounds (a_0= 1.50, b = 0.10)
Temperature of Calculation	20.0^0C

The estimated vapor pressure was 4.5 mm-Hg with a total error factor of 10.0%.
References: (4), Ch. 14 and (5), Ch. 4-6.

E. Henry's Law Constant

Estimation of Henry's Law Constant for styrene was based on use of the vapor pressure - water solubility ratio:

$$H = P_{vp}/S$$

where: H = Henry's Law Constant in atm-m^3/mol
P_{vp} = Vapor pressure in atm
S = Water Solubility in mol/m^3

The input parameters for styrene included:
P_{vp} = 5.0 mm-Hg at 20^0C (measured)
S = 300 mg/L at 20^0C (measured)

Henry's Law Constant was estimated at 2.284×10^{-3} atm-m^3/mol with a total error factor of 1.0.
Reference: (5), Ch. 4-8.

F. Volatilization from Water Estimation

Henry's Law Constant was used to estimate the volatility rate of styrene from water. The procedure in CHEMEST uses Henry's Law Constant to calculate gas and liquid phase mass transfer coefficients and is based on the following equation:

$$C = C_o e^{(-k_v t)} = C_o e^{(-K_L t/Z)}$$

where: C_o = initial concentration (g/cm^3)
k_v = volatilization rate constant
t = time
K_L = mass transfer coefficient for liquid phase
Z = mean depth of water body

This equation was obtained through integration of the following expression:

$$N = K_L (C - P/H)$$

where: N = Flux ($g/cm^2 OS$)
C = Concentration
P = Pressure
H = Henry's Law Constant

A more elaborate derivation of this equation and explanation of the variables can be found in the estimation methods handbook[4]. CHEMEST assigns values to the variables associated with these expressions by requiring wind velocity, water velocity, and depth of water body for the calculation.

The input parameters for the estimation of the volatility rate of styrene were:

Temperature of Calculation	20^0C
Henry's Law Constant	2.284×10^3 atm-m^3/mol (estimated)
Wind Velocity	0.10 m/s
Water Current Velocity	0.10 m/s
Depth of Water Body	0.10 m

Resistance to volatilization associated with transfer of the chemical from the bulk of the water to the interface and associated with presence of surface active agents on water surface were not considered.

An estimated volatilization rate constant of 0.379 $hour^{-1}$ was calculated for styrene with a total error factor of 5.0. References: (4), Ch. 15 and (5), Ch. 4-7.

G. Solubility in Water

The water solubility of styrene was estimated at 25^0C using the octanol/water partition coefficient. The procedure in CHEMEST uses 3 different equations depending on the acidity of the compound and the range of log K_{ow} values. These equations are obtained from those recommended by Lyman[6] and are not listed in the estimation methods handbook[4] nor the CHEMEST manual[5].

The input parameters for estimation of the water solubility of styrene were:

Log K_{ow}	2.95 (measured)
Presence of acid group	No

Equation 12 from Lyman's reference[6] was used to estimate the water solubility of styrene at 246 mg/L with a method error factor of 1.6.
Reference: (5), Ch. 4-1.

H. Soil Adsorption Coefficient
The soil adsorption coefficient for styrene was estimated from the octanol/water partition coefficient. The procedure in CHEMEST uses several regression equations which vary by the chemical classes represented.
The following equation was chosen for styrene based on the chemical class and low error associated with the correlation:

$$\log K_{oc} = 0.937 \log K_{ow} - 0.006$$

The chemical classes represented include aromatics, polynuclear aromatics, triazines, and dinitroaniline herbicides.

The input parameter for the estimation was the measured log K_{ow} value, 2.95. The estimated soil adsorption coefficient was 573 with a total error factor of 1.6.
Reference: (4), Ch. 4.

I. Bioconcentration Factor Estimation
The bioconcentration factor for styrene was estimated from the octanol/water partition coefficient. CHEMEST used the following regression equation:

$$\log BCF = 0.76 \log K_{ow} - 0.23$$

The input parameter was the measured log K_{ow} value, 2.95. The estimated bioconcentration factor was 98 with a total error factor of 3.0.
Reference: (4), Ch. 5.

III. Summary of Physical/Chemical Estimates of Styrene

Physical/Chemical Property	Estimated Value	Measured Value
Octanol/Water Partition Coefficient (Log_{10})	2.87 [a]	(2.95) [b]
Boiling Point	168^0C [c]	(145.2^0C) [e] (145-146^0C) [f]
Melting Point	5.2^0C [c]	(- 30.63^0C) [e] (- 31^0C) [f]
Vapor Pressure	4.5 mm-Hg at 20^0C [c]	(5 mm Hg at 20^0C) [d]
Solubility in Water	246 mg/L at 25^0C [c]	(300 mg/L at 20^0C) [d]
Henry's Law Constant	2.28×10^{-3} atm-m^3/mol [c]	
Rate of Volatilization From Water	0.38 $hour^{-1}$ [c]	
Soil Adsorption Coefficient	573 [c]	
Bioconcentration Factor	98 [c]	

a- MedChem Software Release 3.33, Medicinal Chemistry Project, Pomona College, Claremont, California, 1985.

b- Pomona College, Medicinal Chemistry Project, "Chemical Parameter Data Base," Leo, A.J. and Hansch, C., (Eds.), Seaver Chemistry Laboratory, Claremont, California, July 1, 1977.

c- CHEMEST: A Program for Chemical Estimation, W.J. Lyman and R.J. Potts, (Eds.), Arthur D. Little, Inc., 1985.

d- Verschueren, K., "Handbook of Environmental Data on Organic Chemicals," Van Nostrand Reinhold Company, New York, N.Y., 1977, 659 pp.

e- Weast, R.C., (Ed.), "Handbook of Chemistry and Physics," 57th ed., CRC Press, Cleveland, Ohio, 1976.

f- Health and Environment Laboratories Data, Lab Method No. 1097, 1980.

IV. References

1. "MedChem Software Manual, Release 3.33", Medicinal Chemistry Project, Pomona College, Claremont, California, April 1985.

2. Hansch, C. and Leo, A., Substituent Constants for Correlation Analysis in Chemistry and Biology, Wiley Interscience, New York (1979).

3. Chou, J. and Jurs, P., J. Chem. Inf. Comput. Sci., 19, 172 (1979).

4. Handbook of Chemical Property Estimation Methods, W.J. Lyman, W.F. Reehl and D.H. Rosenblatt (Eds.), McGraw-Hill Book Co., 1982.

5. CHEMEST: A Program for Chemical Estimation, W.J. Lyman and R.J. Potts, (Eds.), Arthur D. Little, Inc., 1985.

6. Lyman, W.J. (Arthur D. Little, Inc.), "Enhancements to CHEMEST Program: Water Solubility," interim report on Task 67 of EPA Contract No. 68-01-6271, U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. (October, 1983).

Appendix 3

Description of Procedures Used to Determine Physical/Chemical Estimates for 2-Vinylpyridine

I. MedChem Software

A. Introduction

The estimate for the octanol/water partition coefficient (K_{ow}) was obtained through the use of Pomona MedChem Software, Release 3.33.[1] The software is based on a procedure which assigns fragment constants to structural subunits. The calculated log K_{ow} is the sum of fragment constants appropriate for the molecule in question.[2] These calculations have been developed into a computer algorithm called CLOGP.[3] The software is a commercially available package from Pomona College.

B. Input Parameter

A chemical nomenclature system, called SMILES, is used to enter the chemical structure as input for the CLOGP algorithm. A SMILES specification uniquely describes the hydrogen suppressed graph of a chemical structure in a way that also defines hydrogen attachments and bond types. More information on SMILES can be obtained from the MedChem Software Manual, Release 3.33. The SMILES input for 2-vinylpyridine was:

c1ccnc(C=C)c1

C. Results

Five types of structural subunits and bonds were defined for the 2-vinylpyridine molecule and are listed with their corresponding fragment values in the following table.

Class	Type	Log (P) Contribution Description	Value
Fragment	#1	Aromatic nitrogen (TYPE 2)	-1.120
Isolating	Carbon	2 Aliphatic isolating carbon(s)	0.390
Isolating	Carbon	5 Aromatic isolating carbon(s)	0.650
Exfragment	Hydrogen	7 Hydrogen(s) on isolating carbons	1.589
Exfragment	Bonds	1 Chain and 0 alicyclic (net)	-0.120

The CLOGP algorithm calculated the log K_{ow} value at 1.389. No error level was determined as all fragment constants were measured values.

II. CHEMEST Software

A. Introduction

The following estimates for 2-vinylpyridine - boiling point, melting point, vapor pressure, Henry's Law Constant, volatilization from water, water solubility, soil adsorption coefficient and bioconcentration factor - were obtained through use of CHEMEST software. CHEMEST is an interactive computer system that provides estimates of environmentally important properties of organic chemicals. The procedures within CHEMEST are based on an estimation methods handbook(4) developed by Arthur D. Little, Inc. CHEMEST is available through online services of Technical Database Services, Inc.(5)

Every CHEMEST output provides information on the method error and, if appropriate, the propagated and total error. Method error, for a given estimation method, is the error that results when all inputs are accurately known. Propagated error is the additional error in the estimate due to the uncertainty in one or more of the inputs which may be estimated values. Total error is a combination of method and propagated error. It is calculated by CHEMEST whenever one or more of the inputs is an estimate with some non-zero. For additional information on the reported errors see reference (5), Chapter 3.2.7.

B. Boiling Point

The Meissner method was used to estimate the normal boiling point of 2-vinylpyridine. It is based on correlating the boiling point with molar refraction (R_D), parachor (P), and a parameter for chemical type (B):

$$T_b = \frac{637\ (R_D)^{1.47} + B}{(P)}$$

where; T_b = boiling point
R_D = molar refraction
P = parachor
B = constant whose value depends on chemical type

CHEMEST calculates R_D using the atomic refraction contribution method of Eisenlohr which consists of summing contributions for each atom, multiple bond and/or substructure in the compound. Parachor is calculated using a similar contribution scheme. The input values for R_D and P were obtained from Table 12-3 and follow:

Molecular Feature	Number	R_D	P
6 member ring	1	0	0.8
-C=C-	3	6.569	37.4
Double bond	1	1.733	19.0
C (singly bound)	1	2.418	9.2
N (in ring)	1	2.840	17.5

Calculated values for R_D and P were 26.7 and 159, respectively. The parameter B is used to adjust the computation of boiling point for compound type. The input value for B was obtained from Table 12-5:

B = -3000 (tertiary amine)

The R_D, P, and B were input into the above equation to calculate an estimated boiling point of 210^{0}C with 5.0% total error.
Reference: (4), Ch. 12.

C. Melting Point
The following equation was used to estimate the melting point of 2-vinylpyridine in the CHEMEST software:

$$T_m = 0.5839\ T_b$$

where: T_m = melting point
T_b = boiling point

The input parameter was the measured boiling point, 160^{0}C. The estimated melting point was calculated at 15.2^{0}C with 8.4% total error.
Reference (5), Ch. 4-9.

D. Vapor Pressure Estimation
The modified Watson method was used to estimate the vapor pressure of 2-vinylpyridine. The method uses the following equation:

$$W\ H_v \quad Z\ W\ H_{vb}\ (3 - 2\ (T/T_b))^m$$

where: $W\ H_v$ = heat of vaporization
$W\ H_{vb}$
T = temperature of calculation
T_b = boiling point
m = constant, calculated from T/T_b ratio by CHEMEST

The heat of vaporization is calculated by CHEMEST using two parameters (a and b) which are associated with the polarity of the compound. The parameters are determined by choosing the compound class that best represents the polarity of the compound.

The input parameter for the estimation of the vapor pressure of 2-vinylpyridine included:

Normal Boiling Point	160^{0}C (measured)
Identification of Physical State	Liquid
Identification of Compound Class	Nonpolar or Slightly Polar Compounds (a = 1.50, b = 0.10)
Temperature of Calculation	25^{0}C

The estimated vapor pressure was 3.7 mm-Hg with a total error factor of 2.0.
References: (4), Ch. 14 and (5), Ch. 4-6.

E. Henry's Law Constant
Estimation of Henry's Law Constant for 2-vinylpyridine was based on use of the vapor pressure - water solubility ratio:

$$H = P_{vp}/S$$

where: H = Henry's Law Constant in atm-m^3/mol
P_{vp} = Vapor pressure in atm
S = Water Solubility in mol/m^3

The input parameters for 2-vinylpyridine included:
P_{vp} = 3.7 mm-Hg at 25^{0}C (estimated)
S = 2.75 x 10^4 mg/L at 20^{0}C (measured)

Henry's Law Constant was estimated at 5.119 x 10^{-5} atm-m^3/mol with a total error factor of 2.0.
Reference: (5), Ch. 4-8.

F. Volatilization from Water Estimation
Henry's Law Constant was used to estimate the volatility rate of 2-vinylpyridine from water. The procedure in CHEMEST uses Henry's Law Constant to calculate gas and liquid phase mass transfer coefficients and is based on the following equation:

$$C = C_o e^{(-k_v t)} = C_o e^{(-K_L t/Z)}$$

where: C_o = initial concentration (g/cm^3)
k_v = volatilization rate constant
t = time
K_L = mass transfer coefficient for liquid phase
Z = mean depth of water body

This equation was obtained through integration of the following expression:

$$N = K_L\ (C - P/H)$$

where: N = Flux ($g/cm^2 OS$)
C = Concentration
P = Pressure
H = Henry's Law Constant

A more elaborate derivation of this equation and explanation of the variables can be found in the estimation methods handbook[(4)]. CHEMEST assigns values to the variables associated with these expressions by requiring wind velocity, water velocity, and depth of water body for the calculation.

The input parameters for the estimation of the volatility rate of 2-vinylpyridine were:

Temperature of Calculation	25^0C
Henry's Law Constant	5.12×10^{-5} $atm\text{-}m^3/mol$ (estimated)
Wind Velocity	0.10 m/s
Water Current Velocity	0.10 m/s
Depth of Water Body	0.10 m

Resistance to volatilization associated with transfer of the chemical from the bulk of the water to the interface and associated with presence of surface active agents on water surface were not considered.

An estimated volatilization rate constant of 0.01910 $hour^{-1}$ was calculated for 2-vinylpyridine with a total error factor of 5.7. References: (4), Ch. 15 and (5), Ch. 4-7.

G. Solubility in Water

The water solubility of 2-vinylpyridine was estimated at 25^0C using the octanol/water partition coefficient. The procedure in

CHEMEST uses 3 different equations depending on the acidity of the compound and the range of log K_{ow} values. These equations are obtained from those recommended by Lyman[6] and are not listed in the estimation methods handbook[4] nor the CHEMEST manual.[5]

The input parameters for estimation of the water solubility of 2-vinylpyridine were:

Log K_{ow}	1.80 (measured)
Presence of acid group	No

Equation 12 from Lyman's reference[6] was used to estimate the water solubility of 2-vinylpyridine at 4.86×10^{3} mg/L with a total error factor of 1.6.
Reference: (5), Ch. 4-1.

H. Soil Adsorption Coefficient

The soil adsorption coefficient for 2-vinylpyridine was estimated from the octanol/water partition coefficient. The procedure in CHEMEST uses several regression equations which vary by the chemical classes represented.

The following equation was chosen for 2-vinylpyridine based on the chemical class and low error associated with the correlation:

$$\log K_{oc} = 1.029 \log K_{ow} - 0.18$$

The chemical classes represented include a variety of insecticides, herbicides, and fungicides.

The input parameter for the estimation was the measured log K_{ow} value, 1.80. The estimated soil adsorption coefficient was 47 with a total error factor of 1.6.
Reference: (4), Ch. 4.

I. Bioconcentration Factor Estimation

The bioconcentration factor for 2-vinylpyridine was estimated from the octanol/water partition coefficient. CHEMEST used the following regression equation:

$$\log BCF = 0.76 \log K_{ow} - 0.23$$

The input parameter was the measured log K_{ow} value, 1.80. The estimated bioconcentration factor was 13 with a total error factor of 3.0.
Reference: (4), Ch. 5.

III. Summary of Physical/Chemical Estimates of 2-Vinylpyridine

Physical/Chemical Property	Estimated Value	Measured Value
Octanol/Water Partition Coefficient (Log_{10})	1.40 [a]	(1.80) [b]
Boiling Point	210^0C [c]	(160^0C) [d]
Melting Point	15.2^0C [c]	
Vapor Pressure	3.7 mm-Hg at 25^0C [c]	(10 mm-Hg at 44.5^0C) [e]
Solubility in Water	4.86×10^3 mg/L [c]	(2.75×10^4 mg/L) [e]
Henry's Law Constant	5.119×10^{-5} atm-m^3/mol [c]	
Rate of Volatilization From Water	0.0191 $hour^{-1}$ [c]	
Soil Adsorption Coefficient	47 [c]	
Bioconcentration Factor	13 [c]	

a- MedChem Software Release 3.33, Medicinal Chemistry Project, Pomona College, Claremont, California, 1985.

b- Health and Environment Laboratories Data, Lab Method No. 1988, (Value determined by HPLC in a method similar to ASTM), 1980.

c- CHEMEST: A Program for Chemical Estimation, W.J. Lyman and R.J. Potts, (Eds.), Arthur D. Little, Inc., 1985.

d- Weast, R. C. and M. J. Astle, (Eds.), Handbook of Chemistry and Physics, 63rd Edition, 1982-1983, p. C-488.

e- Material Safety Data. Reilly Tar & Chemical Corporation, 1510 Market Square Center, 151 North Delaware Street, Indianapolis, Indiana, 3/28/85.

IV. References

1. "MedChem Software Manual, Release 3.33", Medicinal Chemistry Project, Pomona College, Claremont, California, April 1985.

2. Hansch, C. and Leo, A., Substituent Constants for Correlation Analysis in Chemistry and Biology, Wiley Interscience, New York (1979).

3. Chou, J. and Jurs, P., J. Chem. Inf. Comput. Sci., 19, 172 (1979).

4. Handbook of Chemical Property Estimation Methods, W.J. Lyman, W.F. Reehl and D.H. Rosenblatt (Eds.), McGraw-Hill Book Co., 1982.

5. CHEMEST: A Program for Chemical Estimation, W.J. Lyman and R.J. Potts, (Eds.), Arthur D. Little, Inc., 1985.

6. Lyman, W.J. (Arthur D. Little, Inc.), "Enhancements to CHEMEST Program: Water Solubility," interim report on Task 67 of EPA Contract No. 68-01-6271, U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. (October, 1983).

A:ENVIRON1

CATTLE ON FEED: NUMBER OF FEEDLOTS AND MARKETINGS BY SIZE OF FEEDLOT CAPACITY, BY STATES, 1988 1/ 2/

YEAR AND STATE	8000-15999 LOTS	8000-15999 CATTLE MARKETED	16000-31999 LOTS	16000-31999 CATTLE MARKETED	32000 AND OVER LOTS	32000 AND OVER CATTLE MARKETED	TOTAL LOTS	TOTAL CATTLE MARKETED
1988	NO	1000 HEAD	NO	1000 HEAD	NO	1000 HEAD	NO	1000 HEAD
ARIZ			5	112	5	301	18	428
CALIF	11	158	10	187	7	446	59	850
COLO	16	260	9	325	9	1,210	295	2,385
IDAHO	10	160	*4	*315			90	582
ILL							8,400	690
IOWA							16,000	1,845
KANSA	54	1,046	27	1,179	14	1,379	1,900	4,155
MINN							6,000	530
NEBR	43	1,000	14	600	5	460	9,200	5,120
OKLA	8	97	4	200	5	442	230	775
S DAK							4,100	580
TEXAS	44	650	36	1,390	31	2,730	800	5,035
WASH	5	48	*6	*400			70	484
13 ST	198	3,524	113	4,376	80	7,410	47,162	23,459
1989	NO	1000 HEAD	NO	1000 HEAD	NO	1000 HEAD	NO	1000 HEAD
ARIZ			5	113	3	214	15	342
CALIF	11	110	10	217	8	533	55	930
COLO	14	215	10	430	9	1,100	295	2,315
IDAHO	9	135	*4	*358			103	617
ILL							7,900	620
IOWA							16,500	1,775
KANSA	49	1,068	29	1,293	13	1,379	1,900	4,245
MINN							6,000	525
NEBR	51	1,130	17	700	5	410	8,800	5,070
OKLA	7	60	5	250	4	380	250	765
S DAK							4,200	570
TEXAS	42	675	35	1,350	33	2,460	800	4,745
WASH	5	26	*6	*372			65	436
13 ST	193	3,503	119	4,712	79	6,953	46,883	22,955

1/ NUMBER OF FEEDLOTS WITH 1000 HEAD OR MORE CAPACITY IS THE NUMBER OF LOTS OPERATING AT ANYTIME DURING THE YEAR. NUMBER UNDER 1000 HEAD CAPACITY IS THE NUMBER AT THE END OF THE YEAR.
2/ THE 13 STATE TOTALS SHOW THE ACTUAL NUMBER OF FEEDLOTS AND NUMBER OF ANIMALS MARKETED IN EACH SIZE GROUP. THE SUM OF THE NUMBERS SHOWN BY STATES UNDER A SPECIFIED SIZE GROUP MAY OR MAY NOT ADD TO THE 13 STATE TOTAL FOR THAT SIZE GROUP, SINCE FOR SOME STATES SIZE GROUPS ARE COMBINED TO AVOID DISCLOSING INDIVIDUAL OPERATIONS.
* LOTS AND MARKETINGS FROM OTHER SIZE GROUPS ARE INCLUDED TO AVOID DISCLOSING INDIVIDUAL OPERATIONS.

CATTLE AND CALVES - NUMBER ON FEED, JANUARY 1, 1989-90 1/

STATE	1989	1990	1990 AS % OF 1989
AZ	275	253	92
CA	485	490	101
CO	885	900	102
ID	238	200	84
IL	340	310	91
IA	920	980	107
KS	1,460	1,595	109
MN	310	300	97
NE	1,950	2,060	106
OK	305	325	107
SD	260	260	100
TX	2,070	2,100	101
WA	190	170	89
13 STS	9,688	9,943	103
AL	40	30	75
AR	12	10	83
FL	15	20	133
GA	15	13	87
HA	23	16	70
IN	230	235	102
KY	25	20	80
LA	9	9	100
MD	12	12	100
MI	210	220	105
MS	12	8	67
MO	95	90	100
MT	90	80	89
NV	29	28	97
NJ	3	2	67
NM	130	118	91
NY	19	18	95
NC	23	20	87
ND	40	40	100
OH	200	210	105
OR	91	84	92
PA	75	80	107
SC	20	17	85
TN	20	20	100
UT	48	41	85
VA	40	30	75
WV	10	7	70
WI	100	120	120
WY	109	75	69
OTH ST 2/	7	10	143
U.S.	11,440	11,626	102

1/ CATTLE AND CALVES ON FEED ARE ANIMALS FOR SLAUGHTER MARKET BEING FED A FULL RATION OF GRAIN OR OTHER CONCENTRATES AND ARE EXPECTED TO PRODUCE A CARCASS THAT WILL GRADE SELECT OR BETTER. CATTLE AND CALVES ON FEED ARE INCLUDED IN THE CATTLE INVENTORY ESTIMATES BY CLASSES.
2/ OTHER STATES INCLUDES ALASKA, CONNECTICUT, DELAWARE, MAINE, MASSACHUSETTS, NEW HAMPSHIRE, RHODE ISLAND AND VERMONT.

Acc. No. 901465

HEALTH, SAFETY, AND HUMAN FACTORS LABORATORY

Environmental Safety Data Sheet

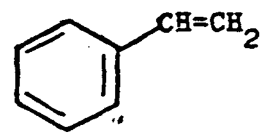
S Reg. No. 100-42-5 HSHFL No. 77-312 Date: 2/ 24/ 78

pirical Formula C_8H_8 Molecular Wt. 104.16

mpound Name Styrene, Vinylbenzene, Ethenylbenzene

nonyms Phenylethylene, Phenethylene, Phenylethene, Cinnamene

ructure:



TSCA Inventory List: ✓ yes ___ no

) Regulatory Status: 1) Currently being tested by NCI for carcinogenicity by Standard Bioassay Protocol as of April 1976.[a] 2) EPA: Selected for Priority Attention as Point Source Effluent Discharge Toxic Pollutant.[1] 3) Among the chemical substances listed in the 19 categories being reviewed for priority testing by the TSCA Interagency Testing Committee for its second-round-of-testing recommendations to the U.S. Environmental Protection Agency.[3]

Environmental Safety Evaluation

) I. Physio-Chemical Properties - Tier "0" Data

( ) Melting Point -30.63°C[4], -31°C[8]
( ) Boiling Point 145.2°C[4], 145-146°C at 760 mm[8]
( ) Vapor Pressure 10 mm @ 30.8°C[4]
( ) Solubility-H_2O 300 mg/l @ 20°C[5,b] <0.1%
( ) pH of 0.1% aqueous solution ______
( ) Solubility-Acetone Soluble[4]; ≥10%[8]
( ) Solubility-3A Alcohol Soluble[4]
( ) Solubility-Octanol ≥0.1%; ≥1.0%[8]
( ) Solubility-Corn Oil ≥10%[8]
( ) pKa-1 ______ Ka ______
Solubility DMSO ≥10%[8]

) II. Environmental Stability

( ) THOD 3.07g/g[5]
( ) COD 2.80, 2.88g/g[5] >1.7g/ml[8,c]
( ) BOD_{20} 87% bio. ox.[2]
( ) BOD_5 0.55-1.95g/g[5]; 2.45g/g (adapted slu
( ) BOD_5/COD 0.19-0.85[5]

( ) T 1/2 - Biological (Activated Sludge T.O.C.) ______

[a] NCI Carcinogenesis bioassay completed as of August 1977.[2]
[b] Solubility-H_2O: 280 mg/l at 15°C; 400 mg/l at 40°C[5]. [c] Incomplete Digestion.

( ) II. Environmental Stability (cont.)

( ) Products of Biodegradation or Biotransformation:

( ) T 1/2 - Photochemical

( ) Products of Photodegradation:

( ) III. Aquatic Toxicity

( ) LC_{50} (24,48,96h)-Fathead-(Soft water)56.7,53.6,46.4 ppm;(Hardwater)62.8,62.: 59.3 ppm[5,6]

( ) LC_{50} - Daphnia magna

( ) LC_{50} - Bluegill (soft water) 25.1 (Lepomis machrochirus)[5,6]

( ) LC_{50} - Goldfish (soft water) 64.7 (Carassius auratus)[5]

( ) LC_{50} - Guppy (soft water) 74.8 (Lebistes reticulatus)[5]

( ) LC_{50} - Fathead minnow, Scud, Snails Daphnia magna All >100 ul/L[8]

( ) Special treatments:

( ) IV. Secondary Waste Treatment Compatibility

( ) IC_{50} >5,000 mg/L[8] Other

Acc. No. 901465

) V. Bioconcentration Potential

( ) WLN 1 U1R

( ) Octanol/water distribution coeff. P=890, log P=2.95[7]

( ) Bioconcentration Factor

( ) T 1/2 - aquatic vertebrate

( ) VI. Phytotoxicity - No effect level

( ) Selenastrum sp.

( ) Germination - Ryegrass 100 μL/L

( ) Germination - Radish 100 μL/L

( ) Germination - Lettuce 100 μL/L

( ) Seedling - Corn

( ) Seedling - Marigold

( ) Seedling - Radish

( ) Seedling - Lettuce

( ) VII. Comments

( ) VIII. References: See attached page.

( ) IX. Environmental Hazard - Tier Testing Ratings (See: HS/HF Laboratory Report, "A Tier Testing Scheme," October, 1977)

	Low (1)	Med. (2)	High (3)
( ) Persistence	1		
( ) Incompatibility	1		
( ) Toxicity		2	
( ) Accumulation		2	

Prepared by:

Philip W. Jenkins, Ph.D.
February 24, 1978

Updated by:

Joseph W. Gorsuch
August 26, 1981

Acc. No. 901465

References for the Environmental Safety Data Sheet on

Styrene; CAS Reg. No. 100-42-5.

1. Christensen, H.E., Ed., "Suspected Carcinogens, 2nd Edition. A Subfile of the NIOSH Registry of Toxic Effects of Chemical Substances," National Institute for Occupational Safety and Health, U.S. Department of Health, Education, and Welfare, Cincinnati, Ohio, December, 1976.

2. Fairchild, E.J., Ed., "Registry of Toxic Effects of Chemical Substances--1978 Edition," National Institute for Occupational Safety and Health, U.S. Department of Health, Education, and Welfare, Cincinnati, Ohio, October, 1978.

3. Bureau of National Affairs, Inc., "ITC Looks at Chemicals Recommended for Inclusion in Next Set of Dossiers," Chemical Regulation Reporter, 1(45), 1575, 1594-7 (January 20, 1978).

4. Weast, R.C., Ed., "Handbook of Chemistry and Physics," 57th ed., CRC Press, Cleveland, Ohio, 1976.

5. Verschueren, K., "Handbook of Environmental Data on Organic Chemicals," Van Nostrand Reinhold Company, New York, N.Y., 1977, 659 pp.

6. Hann, R.W., Jr. and Jensen, P.A., "Water Quality Characteristics of Hazardous Materials," Environmental Engineering Division, Civil Engineering Department, Texas A&M University.

7. Pomona College, Medicinal Chemistry Project, "Chemical Parameter Data Base," Leo, A.J. and Hansch, C., Eds., Seaver Chemistry Laboratory, Claremont, California, July 1, 1977.

8. Health, Safety, and Human Factors Laboratories Data, Lab. No. 77-312. Environmental testing was completed in March, 1980.

ENVIRONMENTAL SAFETY DATA SHEET

TIONS CONCERNING DATA ON THIS SHEET
LD BE REFERRED TO THE ENVIRONMENTAL
CES SECTION, EXTENSION: 85211

HEALTH AND ENVIRONMENT LABORATORIES
ENVIRONMENTAL SCIENCES SECTION

NO.	HAEL NO.	SRID NO.	ACCESSION NO.
	83-0149	Reilly Lot 30912	905464

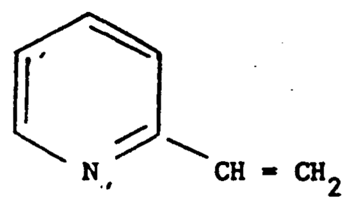
UND NAME

2-Vinylpyridine

NYMS

ECULAR FORMULA C_7H_7N

MOLECULAR WT.



	E=ESTIMATE	LOW (1)	MEDIUM (2)	HIGH (3)
ENVIRONMENTAL FATE	PERSISTENCE			3
	BIOCONCENTRATION	1		
ENVIRONMENTAL EFFECTS	ACUTE AQUATIC EFFECTS			3
	SECONDARY WASTE TREATMENT EFFECTS		2	
	PLANT EFFECTS		2	

PROPERTIES

		OXYGEN DEMAND	
SOLUBILITY: H_2O ≥1.0% <10%	OCTANOL ≥10%	TOD	2.10 g/g
pK_a	K_a	COD	0.742 g/g
MELTING POINT	BOILING POINT	BOD_5	No measurable BOD
VAPOR PRESSURE mm@	°C	BOD_{20}	No measurable BOD

REMARKS The structure was confirmed by IR. The purity was reported as 98.95%, by GC analysis.

BIOCONCENTRATION log P = 1.8.
The log P was estimated by HPLC analysis.

BIODEGRADATION A 21-day biodegradation test utilizing acclimated sludge micro-organisms as the inoculum showed 3.29% degradation of the test article as measured by carbon dioxide evolution.

HOTODEGRADATION

CHEMICAL DEGRADATION

AEL NO.		ACCESSION NO.
83-0149	**ENVIRONMENTAL SAFETY DATA SHEET** **HEALTH AND ENVIRONMENT LABORATORIES** ENVIRONMENTAL SCIENCES SECTION	905464

AQUATIC EFFECTS

LC_{50} - PIMEPHALES PROMELAS (FATHEAD MINNOW)	4.0µL/L[A](1-10µL/L)[B]	LC_{50} - HELISOMA TRIVOLVIS (SNAIL)	3.2µL/L[A](1-10µL/L)[B]
LC_{50} - DAPHNIA MAGNA (WATER FLEA)	3.2µL/L[A](1-10µL/L)[B]	LC_{50} - LUMBRICULUS VARIEGATUS (SEGMENTED WORM)	32µL/L[A](10-100µL/L)[B]
LC_{50} - GAMMARUS FASCIATUS (SIDESWIMMER)	3.2µL/L[A](1-10µL/L)[B]	LC_{50} - ASELLUS INTERMEDIUS (PILLBUG)	3.2µL/L[A](1-10µL/L)[B]
LC_{50} - DUGESIA TIGRINA (FLATWORM)	3.2µL/L[A](1-10µL/L)[B]	LC_{50} - OTHER	

REMARKS

A = nonlinear interpolated 96-hr LC_{50}.
B = the LC_{50} range within the 95% confidence limits.

SECONDARY WASTE TREATMENT COMPATIBILITY

IC_{50} 1200 mg/L

REMARKS

PLANT GROWTH EFFECT NO EFFECT CONCENTRATION

GERMINATION		SEEDLING	
LOLIUM PERENNE (RYEGRASS)	10 µL/L	ZEA MAYS (CORN)	
RAPHANUS SATIVUS (RADISH)	10 µL/L	TAGETES PATULA (MARIGOLD)	
LACTUCA SATIVA (LETTUCE)	10 µL/L	LACTUCA SATIVA (LETTUCE)	
OTHER		RAPHANUS SATIVUS (RADISH)	

REMARKS

REFERENCES, COMMENTS

1) *"Sequential Testing for Chemical Risk Assessment",* *Environmental Risk Analysis For Chemicals*, Van Nostrand Company, 1982, pp. 412-433.

PREPARED BY Joseph W. Gorsuch

DATE November 14, 1986